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GASCON2

A Model to Estimate Ground-level H₂S and SO₂ Concentrations and Consequences from Uncontrolled Sour Gas Releases

October 1990



**CONCORD
ENVIRONMENTAL**

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**A MODEL TO ESTIMATE
GROUND-LEVEL H₂S AND SO₂
CONCENTRATIONS AND CONSEQUENCES FROM
UNCONTROLLED SOUR GAS RELEASES**

CEC.J1692

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GASCON2 SUMMARY

The main body of this report is a technical document and the mathematical relationships may be difficult for a non-specialist to assimilate. The GASCON2 summary has been prepared for those who are interested in obtaining an overview of the report contents without going into the level of detail contained within the main body. For those interested in the details, the GASCON2 summary may be passed over to avoid the repetition of material contained in both the main body and the summary.

1 Background

Natural gas is an extremely important resource for Alberta. In 1985, natural gas production averaged 200 million cubic metres per day and generated \$ 8.9 billion in revenue. Approximately one-half of the natural gas was derived from sour gas which also produced elemental sulphur. In 1985, Alberta supplied about 8.6 million tonnes of sulphur to domestic and foreign markets which generated an additional \$ 957 million in revenue. The production of natural gas and sulphur is expected to continue to play a major role in the Alberta economy for the next few decades.

Implicit in the operation of sour gas facilities is the possibility of an accidental release of sour gas to the atmosphere. For example, during the 14 year period 1975 to 1988, five well blowouts occurred during the drilling of sour wells and seven blowouts occurred during sour gas production. During the same period, at least 30 ruptures were associated with sour gas pipelines. Due to the toxicity of H_2S , a large uncontrolled release upwind and close to a populated area could have serious consequences.

A buffer zone separating sour gas facilities from populated areas and a carefully thought-out emergency response plan can provide a necessary measure of safety when sour gas and residential developments encroach on each other. The difficulty facing planners, regulatory agencies, developers and sour gas facility operators is the determination of buffer and emergency response planning zones that maximize land and resource use without compromising public safety. This difficulty emphasizes the need for a tool which will assist in ensuring that public safety concerns are properly addressed when valuable resource development opportunities are being investigated.

The definition and selection of a concentration criteria can be used to define the edge of a buffer or an emergency response planning zone. The selected value depends on the component of concern (H_2S or SO_2), the exposure period and the corresponding physiological response. For the case of an unignited sour gas release, the toxic constituent of concern is H_2S . If the sour gas release is ignited, then the H_2S is converted to SO_2 which is then the toxic component of concern.

Knowledge of how the concentration changes with downwind distance along with the definition of concentration criteria can serve as a tool to assist land use planners. Mathematical models can be used to estimate ground-level H₂S (or SO₂) concentrations as a function of distance from the uncontrolled sour gas release. Specifically, these models should incorporate H₂S (or SO₂) source conditions which characterize uncontrolled releases and atmospheric dispersion processes.

In Alberta, mathematical dispersion models have been used to estimate ambient H₂S (or SO₂) concentrations which result from uncontrolled sour gas releases. Some of the concepts employed by these models, however, have been identified as being 10 to 20 years out of date with respect to our current understanding of atmospheric behavior. Additionally, these models do not incorporate high velocity jet behavior of the escaping gas near the release point. These deficiencies required the development of a new model specifically designed for uncontrolled releases to ensure that the best available tools are being used to estimate toxic concentrations and consequences resulting from uncontrolled sour gas releases. The availability of a new state-of-the-art model ensures that land use decisions are made on an informed basis.

2 Project Objectives and Organization

The overall objective of this project was the development of a technically sound, model which can be used as a practical tool for estimating downwind distance concentration (H₂S or SO₂) profiles under a wide variety of source and meteorological conditions and the consequences of H₂S emissions to humans. The model was implemented on a computer and went through a detailed evaluation process. This report documents the development and evaluation of the model which is referred to as GASCON2. The GASCON2 model estimates H₂S and SO₂ GAS CONcentrations and CONsequences downwind from an uncontrolled release.

The project described in this report was done under contract to the Energy Resources Conservation Board (ERCB) by Concord Environmental Corporation. A Scientific Advisory Board appointed by the ERCB provided technical advice and peer review throughout the project to assure the scientific acceptability of the overall approach. The development of the system entailed the review of modelling approaches and, in some cases, the development of new approaches to address the unique character of uncontrolled releases.

3 Characteristics of Uncontrolled Releases

To appreciate the factors which determine the downwind distance concentration and consequence profiles, it is instructive to review briefly the behavior of an uncontrolled sour gas release as depicted schematically in Figure 1.

The pressure in the sour gas reservoir is typically 100 times that of the atmosphere. When a well blowout occurs, this high pressure gas is released at the well head to the atmosphere as a high velocity jet. Once in the atmosphere, the sour gas goes through the following processes which can dilute the H_2S concentration by many orders of magnitude:

- Within a few pipe diameters of the release point, the pressure of the escaping gases decreases rapidly to that of the atmosphere.
- The escaping gases are very turbulent and air is drawn in and mixes with the high velocity sour gas jet. This mixing or entrainment of air decreases the velocity of the jet.
- The escaping gases will rise due to vertical momentum and natural buoyancy. The height of the plume will be limited by atmospheric stability and wind speed which will cause the high velocity jet to bend over.
- Turbulent dispersion processes will cause the escaping gases to spread in the lateral and vertical directions as the plume moves downwind. The amount of spreading and dilution depends on atmospheric conditions.

There are a number of alternatives which could alter the situation depicted in Figure 1:

- The escaping gases may either be accidentally or intentionally ignited. The ignition of the plume will shift the concern from H_2S to SO_2 and will increase the height of the plume above the ground due to increased buoyancy.
- The gases may not escape in the vertical direction. A valve failure at the well head, for example, may result in a horizontal release.
- Obstacles such as an overhead drilling platform can remove the vertical momentum from the jet, producing a buoyant cloud which subsequently disperses.
- A mixing height in the atmosphere may limit the vertical movement of the plume reducing the dilution properties of the atmosphere. On the other hand, a plume which has sufficient momentum and/or buoyancy can penetrate the mixed layer and disperse above the mixing height reducing ground-level concentrations.
- The amount of hydrogen sulphide (H_2S) in sour gas can vary considerably from one sour gas pool to another. In instances where wells have not yet been drilled the amount of H_2S in the natural gas can be estimated from the gas delivered from nearby wells producing in the same pool. The other constituents of the gas (methane, propane, ethane, carbon dioxide, nitrogen, etc.) are also important in estimating properties of the sour gas (such as density) and in modelling what takes place when the gas release is ignited. Again, these constituents can be estimated from other wells if the well under consideration has not yet been drilled.

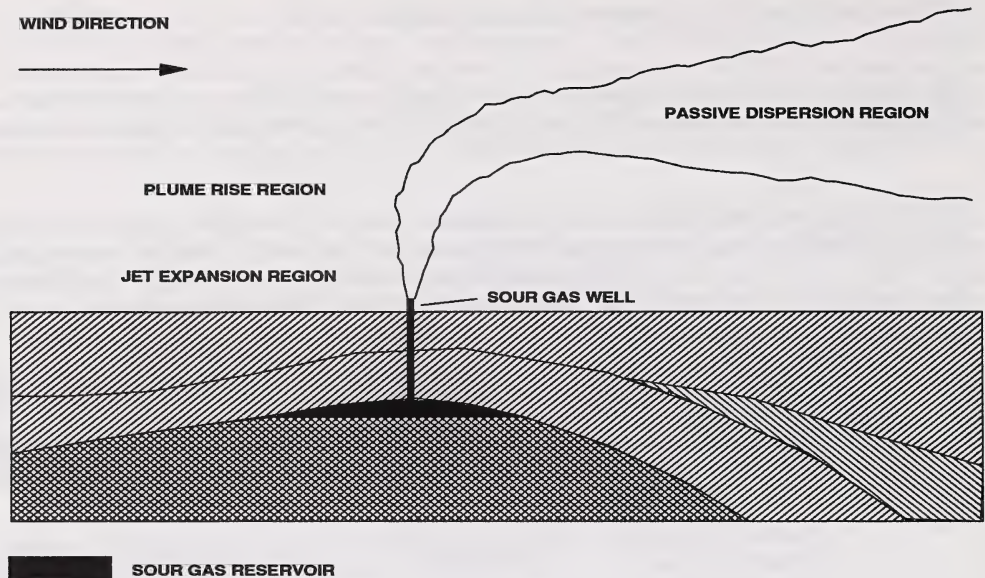


FIGURE 1

Illustration of an Uncontrolled Sour Gas Release.

3.1 Well Blowouts

There are a number of factors which determine the release rate and the initial geometry of escaping gases. For a sour gas well, the surface deliverability of the well will depend on the following flow conditions (Figure 2):

- | | |
|-----------------|---|
| • Casing Flow | Flow up casing or open hole, |
| • Combined Flow | Flow up annulus and drill pipe or tubing, |
| • Annular Flow | Flow up annulus only, and |
| • Tubing Flow | Flow up drill pipe or tubing only. |

The jet may be directed at any angle depending on the nature of the failure. All or part of the jet may be deflected by structures present at the wellhead. Four specific cases were considered for this project (Figure 3):

- | | |
|----------------|-------------------------------------|
| • Downwind Jet | Horizontal jet pointing downwind, |
| • Vertical Jet | Vertical jet, |
| • Upwind Jet | Horizontal jet pointing upwind, and |
| • Cloud | Cloud (jet has lost momentum). |

A well blowout is characterized by a continuous release which can be typically days or weeks in duration.

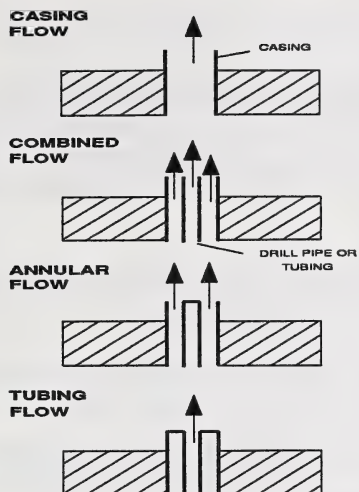


FIGURE 2

Possible Well Flow Scenarios.

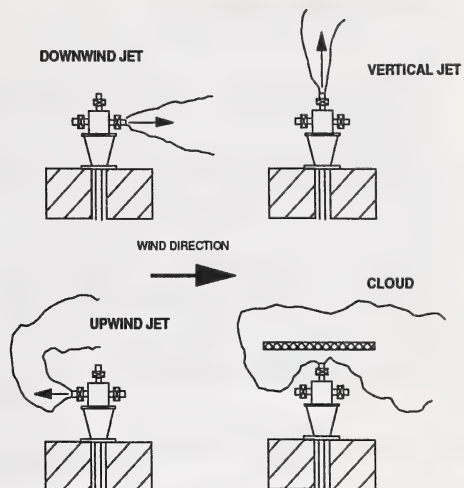


FIGURE 3

Possible Well Release Geometries.

3.2 Pipeline Ruptures

In contrast, a pipeline rupture typically lasts only a few minutes since Emergency Shut Down (ESD) valves isolate the ruptured pipeline segment from the rest of the gas gathering system and limits the amount of sour gas released to the atmosphere. With the presence of ESD valves, the emission rate is characterized by a high initial flow rate which decreases with time as the pipeline is depressurized.

Typical pipeline valve and rupture configurations will lead to different depletion scenarios which will affect the volume and release rate of the sour gas (Figure 4):

- | | |
|-------------------------|---|
| • End Pipe Rupture | Rupture adjacent to an ESD valve, all ESD valves operate as designed. One pipeline segment is depleted. |
| • ESD Valve Failure | Rupture at an ESD valve which fails, all other ESD valves operate as designed. Two pipeline segments are depleted. |
| • Center Pipe Rupture | Rupture between two ESD valves, all ESD valves operate as designed. One pipeline segment is depleted. |
| • Decay to Steady State | Rupture in segment next to wellhead, well ESD valve fails, and all other ESD valves operate as designed (An end rupture is depicted). |

The last scenario will be characterized by a transient release which will decay to the steady state flow driven by the formation pressure through the well. The other scenarios will be characterized by transient releases which will decay to zero.

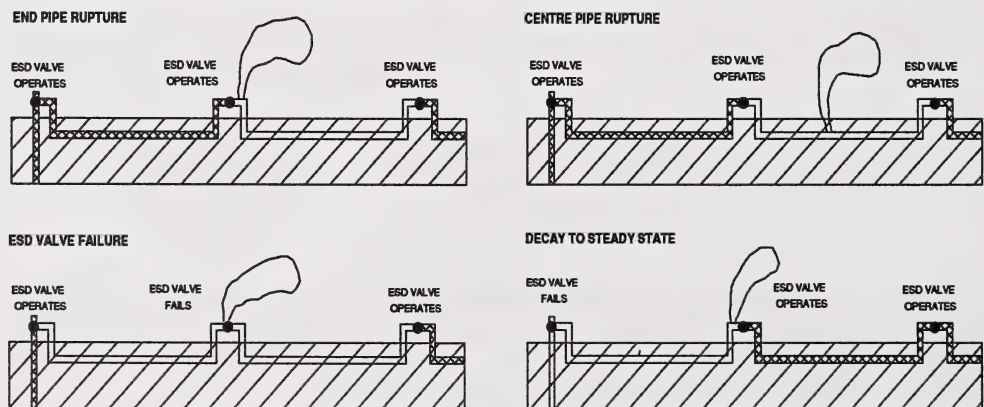


FIGURE 4

Possible Pipeline Rupture Scenarios.

As with a well blowout, the geometry associated with a pipeline rupture will determine the initial behavior of the sour gas in the atmosphere. The cause for the rupture can be external or internal corrosion, metallurgical defects or mechanical (third-party) damage. The release geometries can be broadly categorized as (Figure 5):

- Long Rupture A section of pipe is removed leading to two sources of gas, each being vented from an opening whose cross sectional area is equal to the cross sectional area of the pipe. Two opposing jets could result from such a configuration.
- Short Rupture A short rupture or split can occur on the top, bottom or side of the pipe. The cross sectional area of the opening will be typically equal to the cross sectional area of the pipe.
- Leak Leaks can develop from localized corrosion and are typically pin-sized holes.

Again as is the case for well blowouts, the release geometry can also be described as being an upwind jet, a vertical jet, a downwind jet or a cloud depending on the nature of the release.

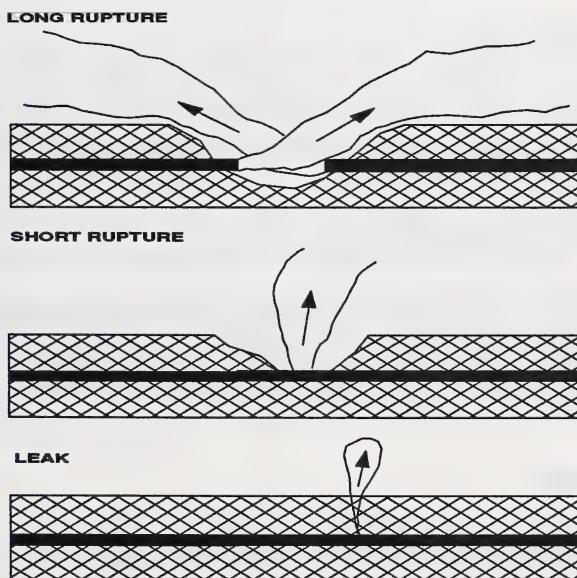


FIGURE 5

Possible Pipeline Release Geometries.

4 Meteorology

The meteorology during an uncontrolled release is perhaps the most important parameter which determines the extent of an exposure zone. The meteorological parameters of importance are:

Wind Speed

Wind speed directly affects the transport of toxic gases in the atmosphere by determining the distance the material moves in a given period of time and the dilution of the material in the along-wind direction. Indirectly, wind speed also affects the rise of the sour gas plume (the faster the wind speed, the lower the plume rise) and the level of turbulence in the atmosphere (the faster the wind speed, the greater the level of turbulence). Increased turbulence levels will increase the dilution of the plume.

Wind Direction

Wind direction determines the direction in which sour gas will be carried and dispersed and the geographical area which will be exposed to the toxic gas.

Temperature

At colder outdoor temperatures the ambient air becomes more dense relative to the sour gas. Because the sour gas is more buoyant in these situations, it will tend to rise higher.

Surface Roughness

Surface roughness is a site-dependent factor which depends on the presence of terrain features such as trees, buildings and crops. An increase in surface roughness will increase the dilution of toxic gas releases. Surface roughness factors are tabulated in many meteorological reference texts under qualitative descriptions of various terrain types.

Stability

Atmospheric stability refers to the level of turbulence in the lowest level of the atmosphere, known as the Planetary Boundary Layer (PBL), within which we live.

Unstable conditions occur when there is significant solar heating of the ground, as one might expect during sunny daytime hours in summer. Under these conditions, large scale convective motions in the form of updrafts and downdrafts are set up in the PBL, causing the rapid dilution of toxic material.

Stable conditions occur when there is cooling of the ground by radiation, as one might expect during the night. Turbulent motions are suppressed in the PBL and toxic gas disperses slowly in these conditions.

Neutral conditions occur when turbulence is neither enhanced (as in unstable conditions) nor suppressed (as in stable conditions). Neutral conditions can occur during transition periods between stable and unstable, and vice versa. They can also occur under high wind conditions.

Mixed Layer Height

This is essentially the height of the PBL in which turbulent mixing takes place. Due to strongly suppressed levels of turbulence at the top of the mixed layer and possible temperature inversions, the mixed layer height can often act as a lid, restricting vertical movement of a sour gas plume. This can reduce the dilution properties of the atmosphere. On the other hand, a plume which has enough momentum or buoyancy to penetrate partially through the mixed layer reduces the amount of toxic gas material to be dispersed within the mixed layer.

The mixed layer height is typically greatest in unstable conditions, when it can be as high as 1 500 to 2 000 metres. The mixed layer height is typically lowest in low wind speed stable conditions, when it can be as low as 50 to 100 metres.

4.1 Meteorological Preprocessor

Wind direction, wind speed and temperature are measured on a routine basis at meteorological stations operated by the Atmospheric Environment Service (AES). AES does not monitor stability, turbulence and mixing heights on a routine basis. Therefore, these parameters have to be estimated from what routine measurements are available and from our understanding of the behavior of the planetary boundary layer. Alternatively, if representative AES stations are not available, then on-site meteorological measurement programs may be initiated during the planning and approval stages of a sour gas facility and for emergency response planning purposes during the operation phase.

A meteorological data preprocessor was developed for this project to estimate atmospheric turbulence levels and mixing height values from routine meteorological observations. This model component is called a preprocessor because it is used before the main component of the GASCON2 model is run. The preprocessor incorporates our current understanding of Planetary Boundary Layer physics.

4.2 Preprocessor Results

For the purposes of illustration, the preprocessor was applied to five years of routine meteorological data from Calgary International Airport for the period January 1 1980 to December 31 1984.

On the average, unstable, neutral and stable conditions were predicted to occur 22, 36 and 42 percent of the time respectively. As expected, unstable conditions occur during day-light hours and stable conditions are primarily associated with night-time conditions. Neutral conditions can be expected any time of the day with a bias to the night-day and day-night transition hours.

Figure 6 compares the preprocessor stability class frequency distributions with those predicted using the more familiar STAR preprocessor approach. The STAR approach predicts unstable, neutral and stable conditions 18, 52 and 30 percent of the time respectively. The preprocessor method predicts more frequent occurrences of unstable conditions. The STAR approach has been found to be biased towards neutral conditions when, in fact, the atmosphere was unstable.

Figure 7 shows the median predicted mixing height values as a function of time of day and season. During the night, the median mixing layer depths are typically 100 m. The mixing depth reaches a maximum between 1600 and 1800 hours (depending on season). During the spring, summer and fall seasons, the preprocessor mixing height results are about one-half the values interpolated for Calgary from seasonal maps prepared from upper air observations.

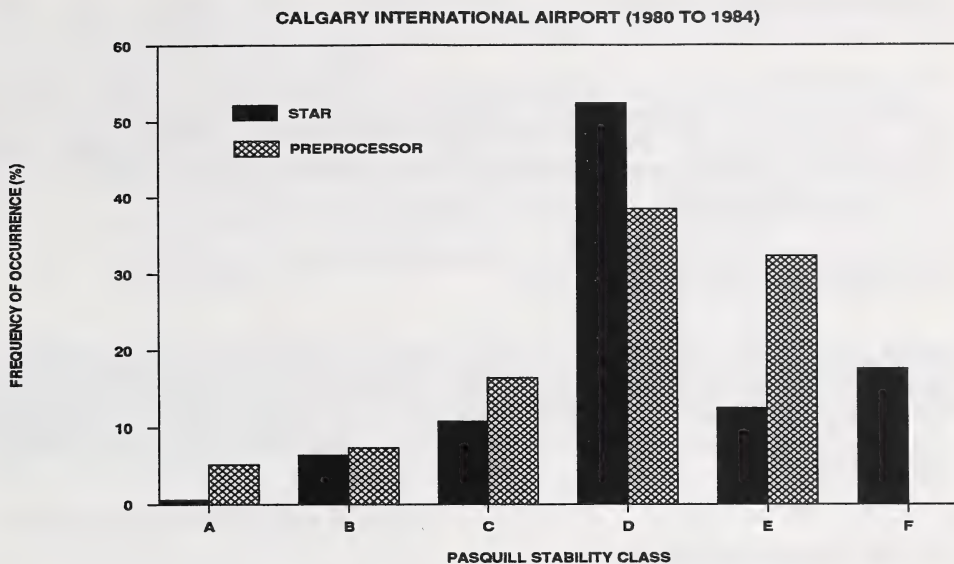


FIGURE 6
Comparison of Pasquill Stability Class Predictions.

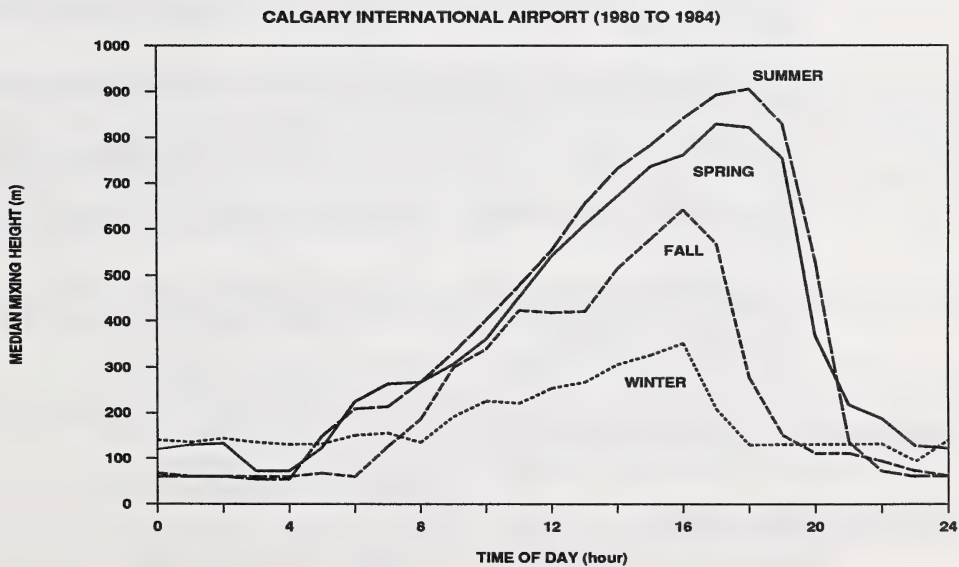


FIGURE 7
Median Predicted Mixing Height as a Function of Season and Time of Day.

5 The GASCON2 Model

The GASCON2 model is used to predict ground-level concentrations of H_2S (or SO_2) as a function of downwind distance and the consequences due to H_2S . The model requires input data characterizing the source release rate, source geometry, meteorology, human vulnerability, exposure time and population density. The GASCON2 model is comprised of six sequential modules.

5.1 Mass Emission Rate Module

The transient release rate of sour gas escaping from a pipeline rupture is estimated using a double exponential blowdown model. This blowdown model has been found to give satisfactory agreement with field data and with more rigorous non-ideal gas models. Transient releases which decay to a non-zero steady-state value can also be simulated in this module.

5.2 Jet Expansion Module

For a well blowout and for virtually the entire duration of a pipeline blowdown, the discharging gas experiences choked flow conditions at rupture exit. The initial behavior of the gas after its release to the atmosphere is treated in five sequential zones:

- The stagnation zone defines the initial conditions at the exit which are determined by the physical properties of the gas, the gas temperature and the area of the release.
- The pressure equalization zone considers the expansion of gas from the sonic underexpanded state to atmospheric pressure.
- The drag zone considers the deceleration of the gas due to impingement with an obstruction.
- The entrainment zone considers the entrainment of ambient air which causes the jet to decelerate.
- The combustion zone considers the potential ignition of the sour gas by accounting for the formation of SO_2 from H_2S and the increased temperature of the combusted gases.

The jet expansion module is used to estimate the effective height of the release, and the initial spread and dilution of the plume.

5.3 Plume Rise Module

As the jet slows down due to the entrainment of ambient air, its behavior begins to resemble that from a conventional industrial stack. The plume will continue to rise due to the vertical momentum which remains in the jet and due to its buoyancy. The latter results from a temperature greater than that of the atmosphere and/or from a molecular mass less than that

of air. The plume rise module estimates the trajectory up to its maximum rise. Due to the nature of uncontrolled releases, the plume rise module incorporates more features than those normally used for industrial stacks:

- the ability to estimate the rise of non-vertical releases,
- the ability to estimate the rise of jets directed into the wind (upwind jets),
- the incorporation of ground effects for horizontally released jets, and
- the definition of additional plume rise termination criteria for the integral plume rise approach.

An integral plume rise model was adapted to handle the above mentioned issues, some of which are unique to uncontrolled releases. The final rise predicted by the plume rise module accounts for mixing height effects and also incorporates the commonly used Briggs' analytical plume rise expressions.

5.4 Transient Dispersion Module

This module provides a time history of downwind concentration from a transient release. An effective mass approach accounts for the nature of transient pipeline releases. The effective mass approach allows the steady-state dispersion equation to be used to estimate ambient concentrations from transient sources. This approach allows for more efficient use of computer resources when compared to other approaches which address transient releases.

5.5 Passive Dispersion

Natural turbulent motions in the atmosphere will cause the plume to spread in the crosswind and vertical directions resulting in further dilution of the plume. The amount of dilution depends on the stability of the atmosphere which can vary with time of day, season, height above the ground and on the presence of limiting mixing layers. The passive dispersion module considers elevated and surface releases, and unstable, neutral and stable atmospheres. Features of this module include:

- A plume penetration submodel which allows for the partial penetration of a plume into the free atmosphere above the mixing layer.
- The use of surface-layer similarity scaling for surface sources and the Gaussian plume model for elevated sources.
- The plume spreads for unstable and stable regimes are allowed to vary continuously according to the turbulence parameters obtained from the meteorological preprocessor.
- An effective turbulence level for stable regimes where turbulence has a strong height dependence, approaching a minimum at the mixing height.

The passive dispersion module estimates plume spreads as given by their standard deviations (σ_y and σ_z) from the appropriate PBL parameters obtained from the meteorological preprocessor. As mentioned above, this allows the turbulence to vary continuously. This is in contrast to commonly used dispersion models which adopt discrete stability classes and corresponding plume spread formulations.

5.6 Fluctuating Toxic Load and Probit Module

This module accounts for two very important factors in the determination of the consequences to people due to an accidental sour gas release of toxic gas concentration. The first factor is the variation in toxic gas concentration ("fluctuating load") due to the natural turbulence in the atmosphere. The second factor is the human susceptibility to toxic gas exposure ("probit analysis"). Together these two factors give an estimate of the likelihood that people exposed to sour gas during an accidental release would be adversely affected.

Variation in Toxic Gas Concentration

Peak concentrations may be several times the average concentration predicted by the passive dispersion module due to the natural turbulent motions of air in the atmosphere. Toxic loads based on average concentrations are not adequate to model adverse effects since the periods of peak concentrations would be severely understated.

GASCON2 incorporates a current model for concentration variability in its treatment of detrimental effects. Because human vulnerability is based on the toxic load, the model is capable of handling the peak periods of toxic gas concentration during the exposure time.

Human Vulnerability to Toxic Gas

Experiments performed on animals and limited documented incidents of accidental human exposures to toxic gas have indicated that both concentration level **and** exposure time are important in defining the potential for an adverse effect. This potential is called the **toxic load**. The toxic load is similar to the concept of **dose**, in that the greater the toxic load that a person is exposed to, the greater his chances of responding adversely. An increase in **either** toxic gas concentration **or** exposure time will increase the toxic load, however the toxic load is more dependent on changes in concentration than exposure time.

The toxic load concept, and its implementation in human vulnerability modelling, is a large step forward in risk assessment methodology. Whereas previous work has made extensive use of critical concentration levels, and the hazard zones defined by them, the approach used in this study accounts for exposure time effects in a realistic way using the toxic load concept.

If a sour gas well blowout were to occur, the toxic effect of H₂S would depend on the length of time people would be exposed to the toxic gas. This exposure time would strongly depend on the delay time for ignition of the sour gas release from a well blowout or the time to deplete a ruptured pipeline segment.

The potential number of people that can be adversely affected by an accidental sour gas release is dependent on the population density (people per square kilometer) in the exposure zone around a sour gas facility.

5.7 Model Limitations

Before applying any model to solve a specific problem, it is important to recognize the limitations imposed by the model assumptions. The following have been identified as limitations to consider when applying GASCON2:

- Limited Pipeline Release Scenarios. Only End Pipe Ruptures or release scenarios which can be considered as the superposition of two or more End Pipe Rupture cases are evaluated.
- Upwind and Downwind Horizontal Jets. The model cannot evaluate horizontal releases which are oriented at some arbitrary angle lateral to the wind (e.g., cross wind releases).
- Combustion Module Gas Chemistry. The chemistry and physics of the ignited plume assume the sour gas to be comprised of methane (CH_4), carbon dioxide (CO_2) and H_2S only. Other gases are accounted for in a limited fashion by the heat of combustion factor.
- No Condensation Effects. The model does not consider the dispersion and deposition of condensate aerosol clouds.
- Steady state atmospheric conditions. The models do not address transient atmospheric phenomena such as the rapid mixing of a plume above the mixing layer by the growth of the mixing height (sometimes called inversion breakup fumigation) or changes in wind direction.
- Travel times less than a few hours. During periods characterized by light winds, disorganized and recirculating wind flows, the usefulness of dispersion models at distances beyond 10 km is limited. A wind speed of 1 m/s and a distance of 10 km correspond to a travel time of 3 hours.
- Averaging periods ranging from a few minutes to a few hours. The model is designed for estimating three-minute to one-hour average H_2S concentrations and up to three-hour average SO_2 concentrations.
- Flat terrain conditions. Significant topographical features such as large hills and deep valleys can have blocking, steering, channeling, or deflecting effects on the plume trajectory. In the model, moderately rough terrain can be accounted for adopting an appropriate surface roughness value.
- Homogeneous terrain. The models do not address changes in the surface characteristics such as roughness with varying downwind distances.
- H_2S Lethality. Consequence estimates are based solely on H_2S inhalation.
- Population Outdoors and Stationary. Model assumes population is outdoors and does not flee to the protection of a building.

- Average Adult Population. Recommended parameters used to describe human response to H₂S are representative of average adults and may not be applicable to sensitive sub-populations (elderly, children, asthmatics).

For some cases where a model limitation may be an important factor, some indication of ground-level concentrations can be obtained by running the model for different cases which bracket the case to be evaluated. For example, the following limitations may be addressed in this manner: Upwind and Downwind Horizontal Jets, Limited Pipeline Release Scenarios and Homogeneous Terrain Conditions.

6 Selected Model Predictions

Well blowout and pipeline rupture concentration and consequence profiles based on reasonable release parameters are presented. The profiles are based on the following model input values:

Well Parameters

- Sour gas release rate of $240 \cdot 10^3 \text{ m}^3/\text{d}$.
- Release diameter of 52.4 mm.
- H_2S concentration of 30% in the sour gas.

Pipeline Parameters

- Pipeline length of 1000 m.
- Pipeline diameter of 154.1 mm.
- Release diameter of 154.1 mm.
- H_2S concentration of 30% in the sour gas.

Atmospheric Parameters

- Stable atmospheric conditions.
- For unignited releases, a wind speed of 1 m/s and a mixing height of 28 m.
- For ignited releases, a wind speed of 3 m/s and a mixing height of 94 m.
- Flat or gently rolling terrain covered by mature agricultural crops.

The above meteorological conditions represent "base case" conditions. For other atmospheric conditions, the predicted concentration values are expected to be less than the values shown in the figures, but some combinations may produce higher results.

Well Blowout Predictions

Figures 8 and 9 show typical predicted H_2S and SO_2 concentrations which could result downwind from a well blowout. The results indicate that the estimated H_2S concentrations are very sensitive to the type of release but SO_2 concentrations are not. For example, the distance to the 100 ppm three-minute average H_2S concentration can be as large as 4 km for a downwind jet. For a vertical jet, the maximum estimated H_2S concentration is considerably less than 100 ppm. The maximum SO_2 concentration of about 1 ppm is much less than that for H_2S .

Figure 12 shows the probability of receiving a lethal toxic load for various well blowout release scenarios. The downwind jet has the highest probability of lethality while the vertical jet and cloud have the lowest. In other words, for a person located 0.5 km downwind of the well blowout, if the release was horizontal, there would be a 100% chance of fatality. But if the release was vertical or a cloud type, the chance of fatality is zero. Fortunately, experience has shown that most releases are of the vertical jet type.

Surface Pipeline Rupture Predictions

Figure 10 shows the transient H_2S concentration-time profiles for selected downwind distances from the release site. At distances of 1 and 2 km, the average H_2S concentration is estimated to exceed 100 ppm for 4 and 5 minutes, respectively. Figure 11 shows typical peak H_2S concentration profiles which could result from a pipeline rupture. The results indicate that the estimated peak concentrations 2 km downwind are not very sensitive to the type of release. However, near the source, downwind jets give the highest concentrations. The differences depend on the relative plume size and elevation above ground. Horizontal jets do not rise as high as clouds and vertical jets and travel a considerable downwind distance before reaching the final rise.

Figure 13 shows that for the base case pipeline, the downwind jet is the only rupture geometry which results in a probability of lethality greater than zero. This type of release could occur from a rupture in above ground pipe at surface facilities. Experience has shown that most pipeline ruptures occur in the buried pipe. Buried pipeline predictions are sensitive to the emission angle. A typical release angle of 45° results in low concentrations of H_2S and no consequences.

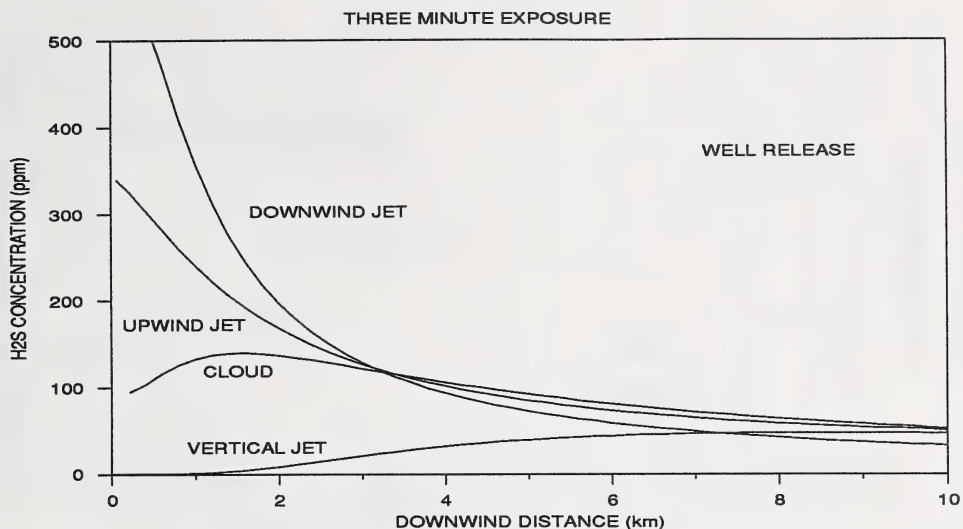


FIGURE 8

Predicted H₂S Concentrations for Selected Well Geometries.

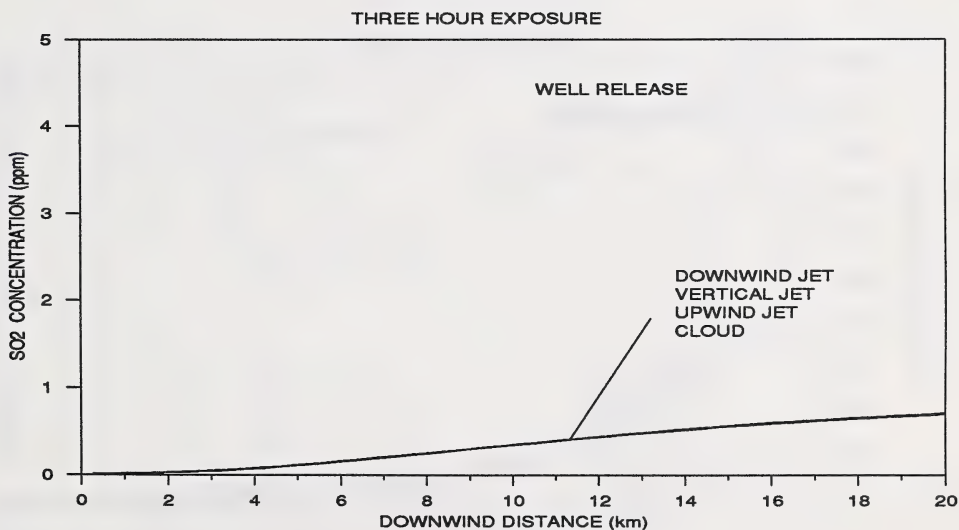


FIGURE 9

Predicted SO₂ Concentrations for Selected Well Geometries.

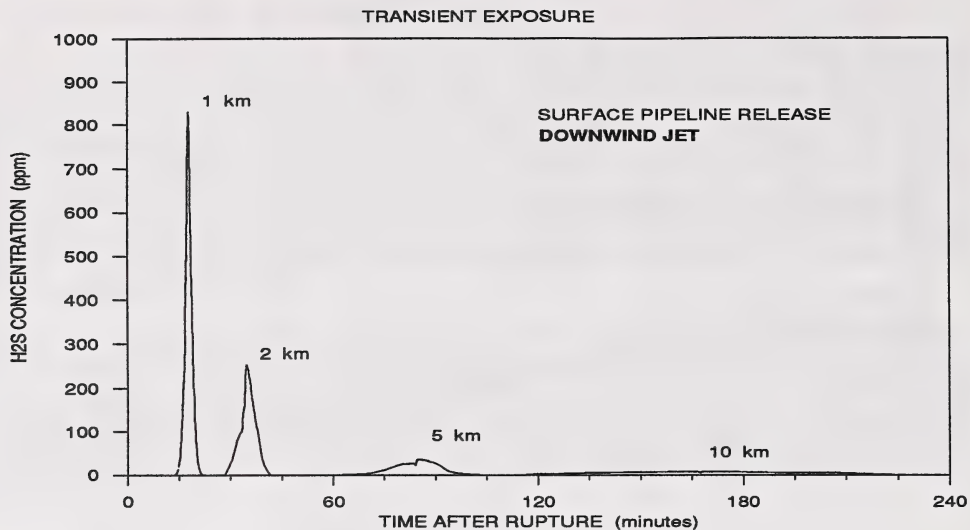


FIGURE 10

Predicted H_2S Concentrations from a Surface Pipeline Rupture as a Function of Time.

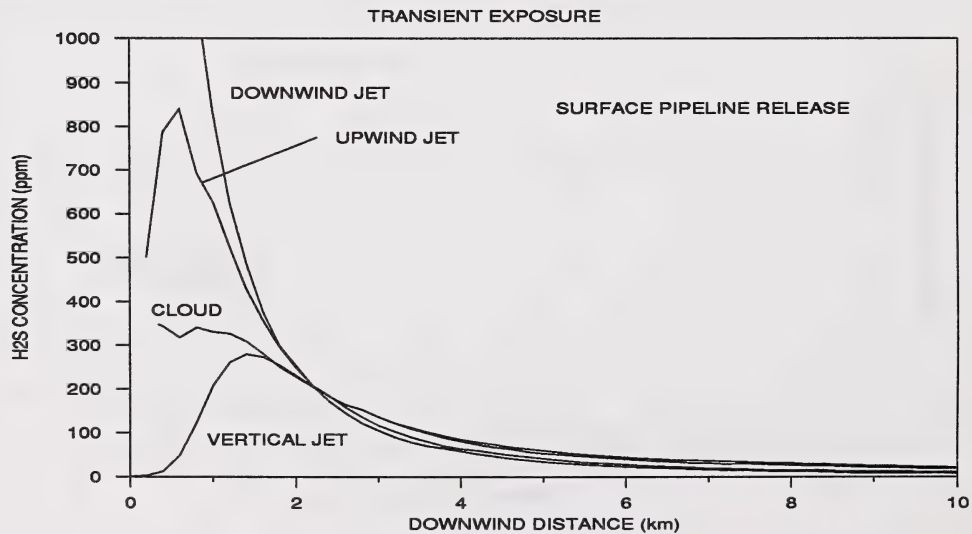


FIGURE 11

Predicted Peak H_2S Concentrations for Selected Surface Pipeline Rupture Geometries.

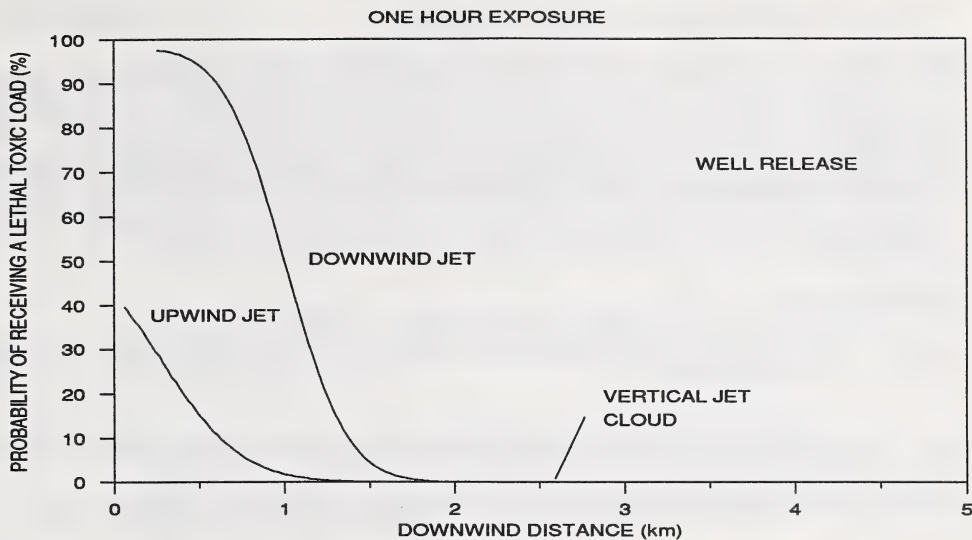


FIGURE 12

Predicted Lethality for Selected Well Geometry Scenarios.

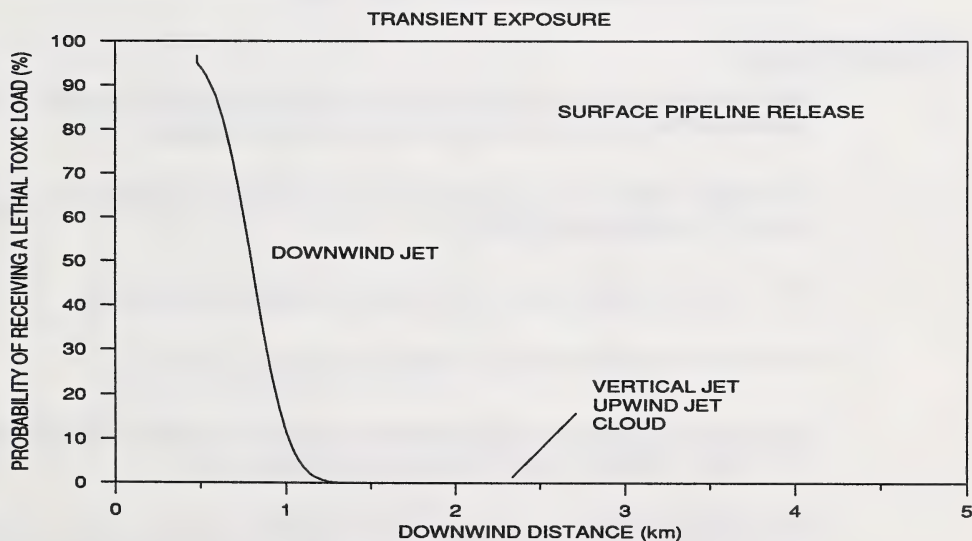


FIGURE 13

Predicted Lethality for Selected Pipeline Rupture Geometries.

7 Model Sensitivity Evaluation Results

Selected source and meteorological input parameters were varied within realistic limits to determine the impact on model predictions of ground-level H₂S and SO₂ concentrations and consequences due to H₂S for a wide range of release and meteorological scenarios. While a wide range of scenarios was considered, it is no doubt possible to conceptualize additional scenarios not addressed specifically in the sensitivity analyses section. For this reason, the following general observations from the model runs conducted to date should be viewed as preliminary:

Well Blowouts

- Horizontal jet releases result in the largest H₂S concentrations and highest consequences.
- Downwind jet releases produce larger concentrations than upwind jet releases.
- Vertical jet releases produce low concentrations due to high plume rise.
- Larger H₂S concentrations and consequences generally result from larger release rates for the unignited case.
- For the plume ignition case, the largest SO₂ concentrations near the well (within 20 km) are associated with smaller release rates.

Pipeline Ruptures

- Predicted concentrations and consequences do not appear to be sensitive to the location of the break in a pipeline segment (for long ruptures).
- The largest predicted concentrations and consequences result from the larger diameter, longer length pipelines.
- Downwind jet releases result in the largest predicted concentrations.
- Vertical jet releases result in the smallest predicted concentrations.
- Increased delay times for the ESD valves to isolate the pipeline segment result in the largest predicted concentrations and consequences.
- Full ruptures (100% hole size) give the highest concentration but a partial rupture of 50% area results in higher consequences due to the effect of exposure time.
- Concentrations and consequences due to buried pipe releases are very sensitive to emission angle. At angles greater than 20° from the horizontal, the downwind effects are negligible.

Meteorology

- Larger H₂S concentrations and consequences are predicted for smaller values of surface roughness.
- Maximum SO₂ concentrations are not sensitive to surface roughness, but the maximum occurs nearer to the well for larger values of surface roughness.
- Predicted concentrations are relatively insensitive to ambient temperatures.
- The largest predicted concentrations and consequences for horizontal releases occur under low wind speed, stable conditions (for unignited H₂S: 1 m/s and for ignited SO₂: 5 m/s).
- For neutral and unstable conditions, the highest predicted concentrations occur relatively close to the source and are associated with moderate to high wind speeds (3 to 15 m/s). Consequences are considerably less under these conditions compared to stable conditions.

In summary, the largest estimated exposure zones for unignited releases are associated with low wind speed stable atmospheric conditions with smooth terrain. For ignited releases, the largest estimated exposure zones are associated with moderate wind speed stable conditions with rough terrain.

8 Uncertainty in Model Predictions

Air quality dispersion model calculations contain uncertainties which can be classified as those arising from reducible errors and those arising from inherent uncertainties. Reducible errors result from errors in source and meteorological input data and from limitations in the model physics. Inherent uncertainties result from the random nature of atmospheric turbulent motions that are responsible for the transport and diffusion processes. To provide a confidence level on the model predictions, it is desirable to quantify these uncertainties. In the absence of observations to allow direct uncertainty analysis, this quantification will require subjective estimates.

Figure 14 shows the combined inherent and irreducible uncertainty for a selected well blowout H₂S release scenario. The band ($\pm 38\%$) represents the smallest uncertainty which can be realistically expected for a given set of input parameters based on estimated uncertainties of these input parameters. This estimated uncertainty is similar to the magnitude of the uncertainties predicted by others and is as good as current technology permits. At first glance, the magnitude of the uncertainties associated with these type of model predictions may not be comforting. It should be kept in mind, however, that concentration values in the atmosphere can vary by many orders of magnitude and that a $\pm 50\%$ uncertainty is better than not having any concentration estimates at all.

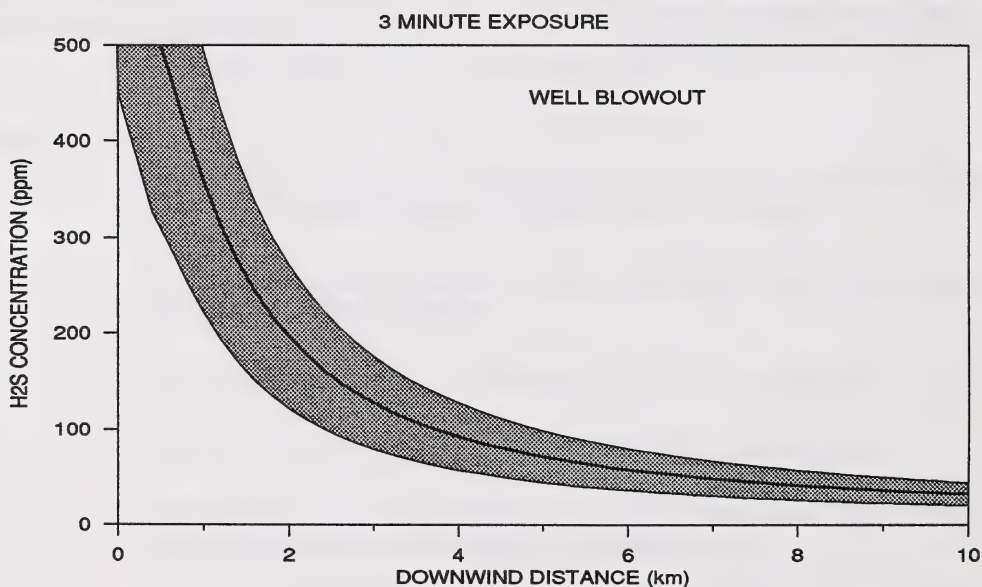


FIGURE 14

Estimated Uncertainty in the Prediction of H₂S Concentrations.

9 Model Comparison

Selected GASCON2 model formulations were compared with other formulations which have been used in Alberta. In particular, the following modules were evaluated:

9.1 Transient Release Rate

The double exponential blowdown model used by GASCON2 was compared to a more rigorous non-isentropic, non-ideal gas model to assess the capability of the former model to predict the high initial release rates.

The double-exponential model gives a somewhat higher release rate during the first 10 seconds following the rupture. It is during this period that the greatest departure from ideal gas behavior can be expected. Based on the comparison between the two models, it was judged acceptable to use the double-exponential model for dispersion modelling purposes.

9.2 Plume Rise

Ambient concentrations are sensitive to the height of the plume above the ground which is the sum of the source height and the plume rise. Final plume rise estimates from the GASCON2 model were compared to those obtained from the Briggs 1969 approach. Vertical unignited and ignited releases were assumed.

The predicted final plume rises for the unignited releases are dominated by the vertical momentum of the plume whereas the ignited releases are dominated by the buoyancy term. The predicted momentum dominated plume rises are generally much less than those which are dominated by buoyancy.

For unstable and neutral conditions, the predicted GASCON2 effective plume height for the portion of the plume which remains within the boundary layer is determined by the plume penetration criterion. These effective plume heights are much less than those predicted by using the Briggs 1969 approach for the complete plume at low wind speeds. At higher wind speeds the effective plume heights (plume rises) predicted by the two approaches are similar. For stable conditions, the predicted GASCON2 effective plume heights are similar but about 20% greater than the Briggs' 1969 approach.

9.3 Plume Spread

Predicted concentrations are also sensitive to the rate at which the plume spreads vertically and horizontally as it moves downwind. The GASCON2 plume spread values were compared to the Pasquill-Smith values used by Alberta Environment in their guideline dispersion models.

For unstable conditions, the use of the GASCON2 plume spreads are expected to produce ambient concentrations similar to, or larger than those associated with the use of the Pasquill-Smith plume spreads for moderate wind speeds of about 3 m/s. For lower wind speeds, the use of the GASCON2 plume spread values are expected to produce ambient concentrations smaller than those associated with the use of the Pasquill-Smith plume spreads.

For neutral conditions, the use of the GASCON2 plume spreads are expected to produce ambient concentrations larger than those associated with the use of the Pasquill-Smith plume spreads.

For stable conditions, the use of the GASCON2 model plume spreads are expected to produce ambient concentrations similar to, or larger than those associated with the use of the Pasquill-Smith plume spreads.

9.4 PLUMES2 Dispersion Model

The Alberta Environment model PLUMES2 was used to calculate H₂S and SO₂ concentrations which result from a vertical steady-state well release. The results were compared to those predicted by GASCON2 for stable atmospheric conditions:

For the unignited release scenario considered, it appears that GASCON2 is more conservative than PLUMES2. That is, GASCON2 predicts larger H₂S concentrations and larger potential hazard zones.

For the ignited release scenario considered, the peak SO₂ concentrations predicted by the models are sensitive to wind speed. For a 2 m/s wind, PLUMES2 predicts a higher peak concentration. For a 3 m/s wind, GASCON2 predicts a higher peak concentration.

9.5 PUFF Dispersion Model

The ERCB model is used to calculate H₂S concentrations which may result from a transient pipeline release. The results were compared to those predicted by GASCON2. Release-rate and plume-height profiles are required as input for PUFF and were obtained from GASCON2.

The downwind H₂S concentration profiles are similar for both models. The main differences occur near the release point. The similarity of the two profiles is not surprising since the GASCON2 release-rate and plume-height profiles were used as input into the PUFF model.

10 Comparison With Observations

Downwind H_2S and SO_2 concentrations are available from three publicized well blowouts in Alberta (Lodgepole, Claresholm and Rainbow Lake). GASCON2 model predictions were compared to observations associated with these blowouts. Due to the severe limitations of the data associated with each blowout, the comparison exercise should NOT be viewed as a model verification or validation exercise. The comparison exercise should only be viewed as providing a preliminary indication of the model performance.

Figure 15 compares model predictions with the observations. Mobile H_2S observations have been normalized to a three minute average while those from stationary monitors have been normalized to a one hour averaging period using the power law relationship. Stationary SO_2 observations were normalized from a one hour average to a three hour average.

The diagonal lines on the figure represent the perfect 1:1 correlation (perfect agreement) and the "factor of two" envelope. Predicted values are scattered both above and below the 1:1 line. Thirty-seven predicted values are above the 1:1 line (overprediction) and 12 predicted values are below the 1:1 line (underprediction) with one in perfect agreement.

In conclusion, the model appears (on the basis of limited data) to significantly overpredict for the downwind distances where observations were available (> 10 km).

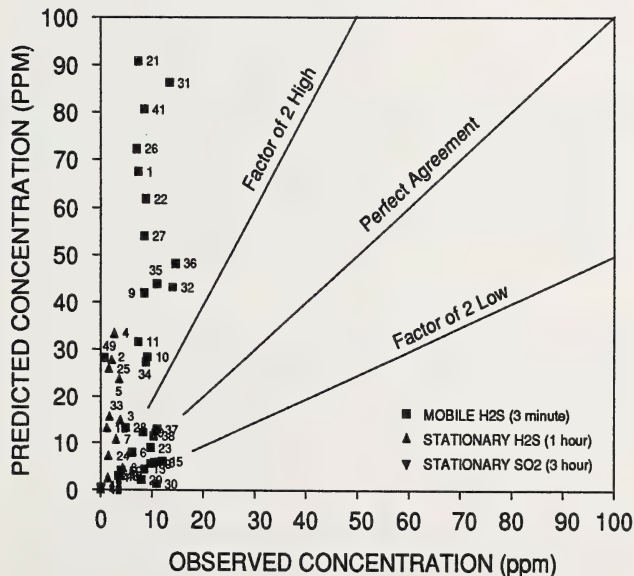


FIGURE 15

Predicted H_2S and SO_2 Concentrations for Selected Well Blowout Observations.

11 Conclusions

The GASCON2 model incorporates our current knowledge to produce an application oriented model which can be used to estimate H_2S and SO_2 concentrations and consequences due to H_2S , which result from uncontrolled sour gas releases with more confidence than previously available models. The model can be used as a tool to help ensure that public safety concerns in the vicinity of sour gas developments are addressed in a rigorous manner.

1 INTRODUCTION

Concord Environmental Corporation has developed a computer-based model which can be used to estimate potential exposure zones associated with an uncontrolled release of sour gas. The uncontrolled release scenarios specifically addressed by the model include unignited releases (H_2S emission) associated with well blowouts and pipeline ruptures and ignited releases (SO_2 emission) associated with well blowouts. The model was designed to serve as a tool to estimate buffer and emergency response planning zones associated with sour gas facilities in Alberta.

The model estimates downwind distance concentration profiles, potential hazard zones, the probabilities that the concentrations of H_2S occurring downwind are lethal, and the potential number of fatalities due to the uncontrolled release.

This project was conducted on behalf of the Energy Resources Conservation Board as part of their continuing evaluation of sour gas development and public safety concerns. A Scientific Advisory Board appointed by the Energy Resources Conservation Board provided a technical and peer review component throughout the project to assure the scientific acceptability of the overall approach and the specific assumptions embodied in the modelling system. The development of the system entailed the review of current modelling approaches and, in some cases, the development of new approaches to address the unique character of uncontrolled releases.

1.1 Background

Natural gas is an extremely important resource for Alberta. In 1985, natural gas production averaged 200 million cubic metres per day and generated \$ 8.9 billion in revenue. Somewhat more than half of the natural gas was derived from sour gas which also produced elemental sulphur. In 1985, Alberta supplied about 8.6 million tonnes of sulphur to domestic and foreign markets which generated an additional \$ 957 million in revenue. The production of natural gas and sulphur is expected to continue to play a major role in the Alberta economy for the next few decades (ERCB, 1986).

Sour gas, however, is a resource to be treated with respect. The term "sour" refers to the hydrogen sulphide (H_2S) content of the gas. H_2S is a colourless gas with a characteristic odour of rotten eggs. High concentrations (1000 ppm by volume) of H_2S are extremely toxic and can result in immediate death; low concentrations (20 to 50 ppm by volume) may be extremely irritating to the lungs, nose, throat and eyes (Occupational Health and Safety Division, 1985).

Sour gas produced from a well is transported under pressure in a pipeline to a processing plant where the H_2S is converted to elemental sulphur. Implicit in the operation of sour gas facilities is the possibility of an accidental release of sour gas to the atmosphere. For example, during the 14 year period 1975 to 1988, five well blowouts occurred during the drilling of sour wells and seven blowouts occurred during sour gas production. During the same period, at least 30 ruptures were associated with sour gas pipelines. Due to the toxicity of H_2S , a large uncontrolled release upwind of and close to a populated area could have serious consequences.

A buffer zone separating sour gas facilities from populated areas and a carefully thought-out emergency response plan can provide a necessary measure of safety when sour gas and residential developments encroach on each other. The difficulty facing planners, regulatory agencies, developers and sour gas facility operators is the determination of buffer and emergency response planning zones that maximize land and resource use without compromising public safety.

The public, in addition, has justifiably become increasingly concerned over the safety of industrial facilities in general and sour gas facilities in particular. Recent uncontrolled toxic releases from industrial operations have included:

- Western Co-op Fertilizer gas release (April 1987)
- Bhopal chemical release (December 1984)
- Mississauga chemical transportation release (November 1979)

Recent uncontrolled releases of H_2S from sour gas facilities in Alberta have included:

- Rainbow Lake well blowout (December 1985)
- Claresholm well blowout (September 1984)
- Lodgepole well blowout (October 1982)

The above mentioned accidental releases, coupled with implicit assurances that a failure could not occur, emphasize the need for a tool which can be used to determine, with confidence, buffer and emergency response planning zones. The development of such a tool will assist in ensuring that public safety concerns are properly addressed when valuable resource development opportunities are being investigated.

A hazard assessment model allows one to examine realistically possible uncontrolled sour gas release events and also to determine the worst case scenario for ground-level toxic gas concentrations. The trouble with "realistically possible" events is that "conceivable" events are sometimes extremely unlikely events. Also, it is generally not practical to make planning decisions based on "worst-case" outcomes; if people adopted worst cases as the basis for their decision-making, nothing would ever get done for fear of the possible outcomes. Almost any activity that would come to mind would be fraught with disastrously possible (but unlikely) consequences.

It is important to recognize that a worst-case outcome cannot of itself provide a rational measure of danger to the public; it must be viewed in the context of the chances of such a worst-case outcome occurring. When one speaks of the chances of an adverse outcome occurring, one is referring to **risk**.

Risk is an inseparable part of life; each person lives with the knowledge that an unexpected event may intervene at any time in his or her life and that some events are more likely to happen (i.e., are riskier) than others.

Risk analysis of environmental hazards has developed as a system for estimating the quantitative (numerical) probabilities associated with events and their consequences to the people, machines, buildings or natural environment affected by those events. Risk analysis is intended to provide data for decision-making with regard to activities or technologies that entail potentially significant levels of risk. Quantitative risk estimates for a technological activity can be evaluated along with costs, benefits, risks of alternatives and mitigating

measures in the decision-making process. The process of developing the risk values is generally called risk assessment and judging the risk values along with the qualifying factors is generally referred to as risk management.

In order that regulatory agencies can make rational decisions regarding safety precautions and emergency planning, and in order that members of the public can follow the rationale for those decisions, it is best that quantifiable estimates of the risk to public safety be made available to all interested parties. Once a measure of the risk posed by a sour gas facility is in hand, mitigative measures can be assessed in a quantitative manner, and the estimated level of risk can be incorporated into the decision-making process.

In simple terms, risk can be quantified as frequency times consequence: how often an event is expected to occur times the estimated adverse outcome of the event. This report assumes the event has occurred and determines the adverse outcome or consequences (probability of lethality). The frequency of the uncontrolled sour gas releases is discussed in Volume 6 (Alp *et al.* 1990).

1.2 Modelling Approach

A mathematical model which simulates the release and dilution of H_2S in the atmosphere can be used to assess the impact of ambient H_2S (or SO_2) concentrations resulting from uncontrolled sour gas releases. Specifically, the model should incorporate concentration and dose values of concern, source conditions which characterize uncontrolled releases and atmospheric dispersion processes.

For the case of an unignited sour gas release, the toxic constituent of concern is H_2S . If the sour gas release is ignited, then the H_2S is converted to SO_2 which is then the toxic component of concern. The selection of the concentration criteria is dependent on the component of concern, the exposure time and the corresponding physiological response. The concentration level alone is not an adequate measure of lethality. Exposure time is also important because toxic gas has a cumulative adverse effect with time on human (and animal metabolism). The approach used should account for concentration and time to estimate the hazard.

Much of the modelling efforts by the air pollution regulatory community have focused on controlled releases from elevated sources (stacks). Release conditions, gas flow rates and gas compositions resulting from stacks are usually known. In contrast, the source characteristics associated with an accidental uncontrolled release of sour gas are not known in advance. The release characteristics will be dependent on the events causing the accident. For this reason, considerable care and effort are required to determine the unique characteristics of an uncontrolled sour gas release.

Air quality simulation models provide a scientific means of relating source characteristics, emissions and meteorological conditions to ambient concentration values. These models use mathematical algorithms which simulate dilution (dispersion) processes in the atmosphere. Regulatory agencies have long recognized the usefulness of air quality models and have relied on them for controlling and solving industrial air pollution problems.

In Alberta, a number of models have been used to estimate ambient concentrations which may result from uncontrolled releases. Two of the models were explicitly designed to handle transient releases associated with pipeline ruptures:

- An integrated PUFF model developed by the ERCB to estimate ground-level H₂S concentrations. This model addresses plume dispersion processes only and does not estimate release rates or plume heights associated with the transient pipeline release (ERCB, 1979).
- A RISK model developed by Alberta Environment to estimate ground-level H₂S concentrations and the probability of receiving a lethal dose at a given location (Choukalos, 1980).

Three other models which have been applied to steady state well releases are the Alberta Environment (1988) guideline models which are primarily used for the design of stacks:

- STACKS2 can be used to estimate ambient H₂S concentrations under plume trapping conditions.
- FLARES2 can be used to estimate ambient SO₂ concentrations under plume trapping conditions.
- PLUMES2 can be used to estimate ambient H₂S concentrations for a wide range of meteorological conditions.

The concepts employed by the above models (e.g., the Pasquill-Gifford dispersion curves and the Pasquill-Turner method of estimating atmospheric stability) have been identified as being 10 to 20 years out of date with respect to our current understanding of atmospheric behavior (Weil, 1985). The above models also do not incorporate high velocity jet behavior of the escaping gas near the release point.

The incorporation of our current understanding of plume dispersion processes and the behavior of the escaping gases near the release point require the development of a model specifically designed for uncontrolled releases. This will ensure that the best available tools are being used to estimate H₂S and SO₂ concentrations resulting from uncontrolled sour gas releases.

Exposure time is particularly important in sour gas releases into the atmosphere for two reasons:

- First, some uncontrolled releases are extremely transient, lasting only a few minutes; the effects of potentially high peaks of concentration of short duration may be offset by the short exposure time.
- Second, dispersion models predict time-averaged concentrations, but in reality turbulent fluctuations in the atmosphere can produce large and relatively rapid swings about the average concentration level; these large variations could produce large momentary concentration peaks which may be large enough to pose a threat to human life.

An appropriate measure of the potential for lethality is the **toxic load**, a combination of toxic gas concentration and exposure time. The toxic load concept is the foundation of the analysis used in the consequence model. Two scientific concepts: **probit analysis** and **fluctuating toxic load** analysis have been employed to estimate the probability of lethality and potential fatalities in an innovative and physically comprehensive manner.

For a given release event, defined by the sour gas release emission, release geometry and meteorological conditions which give rise to downwind concentrations of toxic gas, the probit analysis and fluctuating load analysis permit the lethality of the H₂S concentrations to be quantified. To arrive at the risk to the human population in the vicinity of the release, however, one must quantify the frequency of that release event occurring (Alp *et al.* 1990).

1.3 Modelling Objectives

The overall objective of this project is the development of a model which can be used as a practical tool for estimating downwind distance concentration profiles of H₂S or SO₂ and the consequences due to H₂S exposure under a wide variety of source and meteorological conditions. To meet this overall objective, the following sub-objectives were defined:

- Determine the different well blowout and pipeline rupture release scenarios which could affect the flow rate and source geometry,
- Select a technically sound model approach based on a scientific examination of alternate approaches,
- Implement this model approach on a computer,
- Evaluate the model performance through sensitivity analyses, uncertainty analyses, comparison with other models and comparison with observed concentration data,
- Identify the meteorological and source conditions which are likely to produce the largest exposure zones, and
- Provide a scientific reference document for the selected model approach and performance evaluation.

This report fulfills the last objective by documenting the development and evaluation of the model which will be referred to as **GASCON2**. The **GASCON2** model estimates H₂S and SO₂, **GAS CON**centrations and **CON**sequences downwind from an uncontrolled release.

1.4 Project Organization

The project described in this report was done under contract to the Energy Resources Conservation Board (ERCB) by Concord Environmental Corporation. A Scientific Advisory Board was appointed by the ERCB to provide a technical and peer review of the project.

The **Environment Protection Department** of the **ERCB** was responsible for the coordination of the project. The Environment Protection Department provides information and advice to other operating departments within the ERCB on air and water quality, land management, and emergency response planning concerns. The responsibilities of the ERCB in Alberta include:

- Approving applications for new energy projects,
- Regulating the operation of existing energy facilities, and
- Providing advice and information to industry, the public and government.

The ERCB works closely with Alberta Environment to ensure that environmental impacts resulting from the operation of proposed and existing energy developments are acceptable.

Concord Environmental Corporation is a professional services firm with expertise in environmental sciences and technology. Concord has offices in Toronto, Ottawa, Calgary and Vancouver. Concord has considerable experience in the development and application of models to help resolve air pollution problems. Two examples include:

- The development of a dispersion model to predict hazard zones created by toxic or flammable heavy gas releases (Alp, 1985).
- The development of a modelling system for simulating long range transport and acidic deposition (commonly called acid rain) (USEPA and AES, 1987).

Concord retained the services of Bissett Resource Consultants Ltd. and Mr. V.P. Milo. Bissett Resource Consultants, a Calgary based petroleum engineering firm, has field and management expertise in the various phases of sour gas wells: drilling, completions, workovers and production. Mr. V.P. Milo's main area of expertise is in the selection of materials and the control of corrosion for sour gas facilities. Most of this experience was gained while employed by a major energy company for 28 years.

Specifically, the Concord project team has expertise in the following areas required for the review and development of the modelling system:

- Fluid flow,
- Dispersion meteorology,
- Mathematical modelling,
- Toxic chemicals,
- Sour gas operations, and
- Risk Assessment and Management

A **Scientific Advisory Board** appointed by, and reporting to, the Energy Resources Conservation Board, provided a technical and peer review component throughout the project to assure the scientific acceptability of the overall approach and the specific assumptions embodied in the modelling system. Members of this Board include:

- Dr. D. Wilson is a professor in the Department of Mechanical Engineering at the University of Alberta. His research activities relate to the following areas: turbulent fluid dynamics, atmospheric dispersion, residential energy losses from air infiltration, turbulent concentration fluctuations and pipeline rupture assessments.

- Mr. R. Angle is the Section Head of Scientific Applications, Air Quality Control Branch, Alberta Environment. Mr. Angle is a meteorologist with experience in the following areas: acid deposition, air pollution modelling, risk analysis, atmospheric chemistry, instrumentation guidelines and air quality impact assessments.
- Dr. R. Purvis is Manager of the Special Studies Group at the Energy Resources Conservation Board. He has experience in drilling, production and reservoir engineering in western Canada. His current work involves the development and implementation of computer software to engineering applications.
- Dr. R. Rogers is president of Toxcon Consulting Ltd. located in Sherwood Park. He has experience in the areas of environmental and industrial toxicology and occupational health. He is also an instructor at Concordia College.

The expertise of the Scientific Advisory Board members address the major technical aspects associated with evaluating the impact of uncontrolled sour gas releases.



2 CONTROLLING PARAMETERS

There are several important factors which determine the potential exposure zones from uncontrolled sour gas releases:

- Initial H_2S concentration in the escaping gases,
- Ignition of the escaping gases to produce SO_2 instead of H_2S ,
- Source release geometry which define the orientation, plume rise and initial dilution of the escaping gases,
- Emission rate of the escaping gases as a function of time,
- Meteorological conditions during the release which affect the transport, rise and dispersion of the escaping gases,
- Critical concentration level used to define the extent of the hazard zone,
- Exposure time,
- Human vulnerability criteria,
- Toxic load accounting for fluctuations in concentration, and
- Population density.

The schematic illustrating the inter-relationships among the controlling factors, the modelling framework and the determination of the concentration profiles, hazard zones, probability of lethality and potential fatalities is given in Figure 2.1.

Each controlling parameter can assume a range of physically possible values. A specific combination of a unique set of source and meteorological parameters is defined as a **release scenario**. For any release scenario, a **hazard zone** is defined as the point where the ambient (H_2S or SO_2) concentration has been diluted from the initial concentration to the defined concentration criteria (H_2S or SO_2). As depicted in Figure 2.2, the hazard zone can be thought of as an ellipsoid shaped area whose major axis is oriented along the direction of the wind. The maximum length of the major axis is along the plume centreline.

Since the wind can blow from any direction, a **potential hazard zone** can be defined by a circle whose radius is given by the major axis of the hazard zone. Through the consideration of a wide range of release scenarios, the maximum potential hazard zone may be determined. This maximum potential hazard zone may then be used to assist in the determination of buffer or emergency response planning areas.

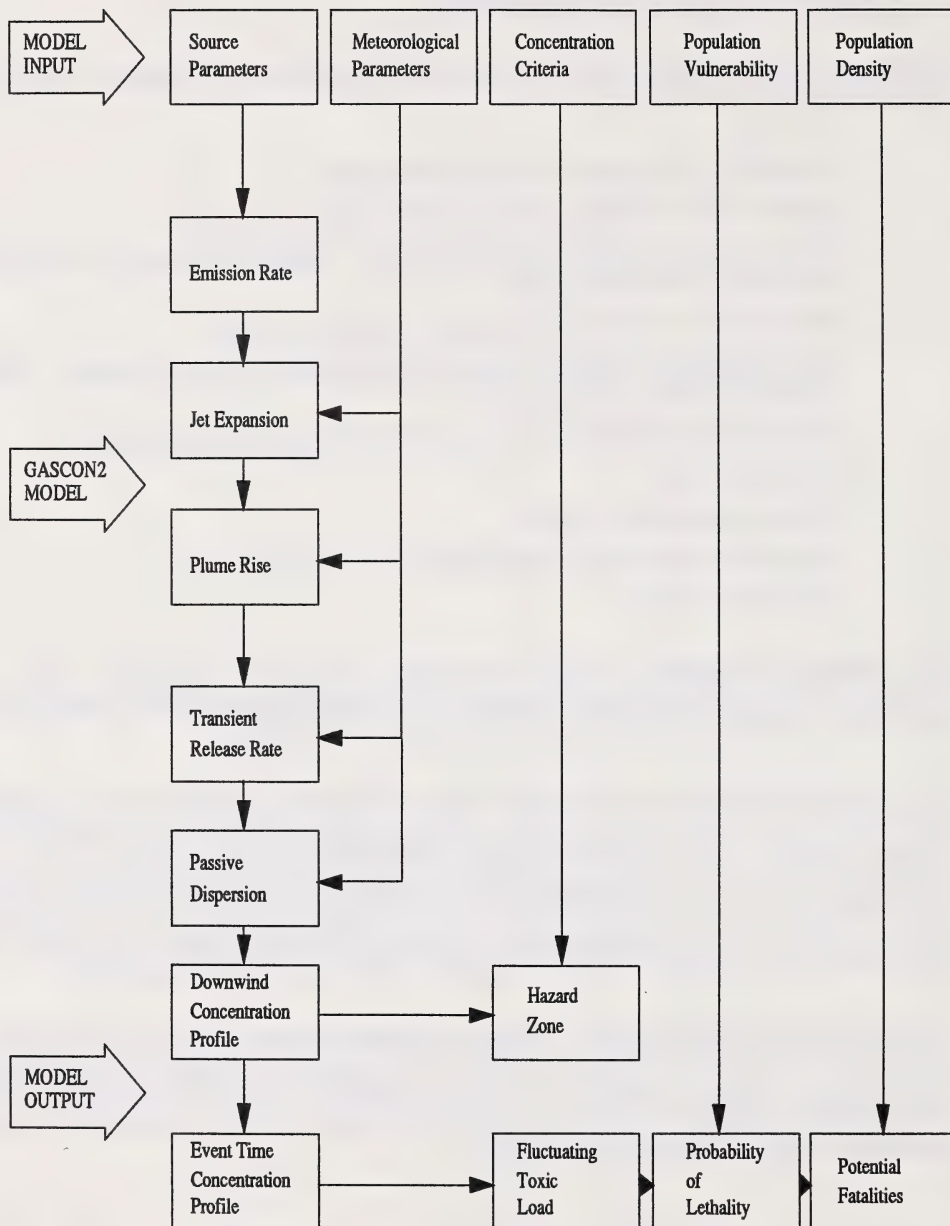


FIGURE 2.1
Schematic of GASCON2 Model Components.

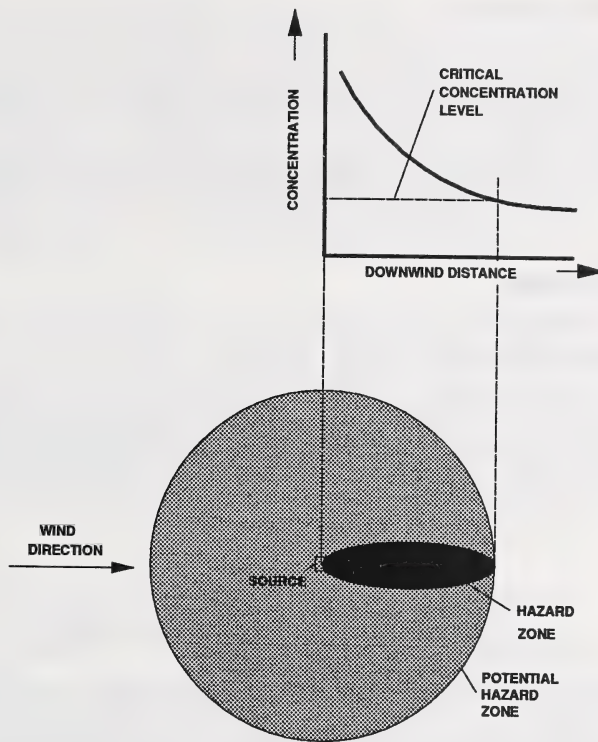


FIGURE 2.2
Hazard Zone Concept.

2.1 Source Parameters

Releases from wells and pipelines approximate the behavior of high velocity jets. The resulting gas cloud may also be buoyant (less dense than the ambient air), depending on the composition and temperature of the sour gas, and on whether or not ignition has taken place. For both wells and pipelines, a number of alternate flow rates and geometries are possible depending on the nature of the well or pipeline failure.

2.1.1 Well Blowout

The various phases associated with the development of a gas well are: general drilling, completion and workover, and production. The potential sour gas flow rate from the well will also be dependent on whether or not the formation has been stimulated by chemical or hydraulic fracture treatment. Table 2.1 illustrates the various activities associated with the development of a well.

Table 2.1
Activities During the Lifetime of a Well.

PHASE	ACTIVITY	FORMATION
General Drilling	Drilling Tripping Coring Logging Testing Casing	Unstimulated
Completion and Workover	Perforating Stimulating Tripping	
Production	Producing	Stimulated

The general drilling, completion and workover activities involve the presence of personnel and equipment at the wellsite. During the production phase, operating personnel attend to the well facilities on an as required basis.

Figure 2.3 illustrates the various flow alternatives and the associated activities. The flow of fluids from the formation will be influenced by the presence of drill pipe or tubing in the casing. During the various activities, the fluid can flow through the casing, annulus and/or the drill pipe or tubing. These four cases, as summarized in Figure 2.3, are:

- | | |
|-----------------|---|
| • Casing Flow | Flow up casing or open hole, |
| • Combined Flow | Flow up annulus and drill pipe or tubing, |
| • Annular Flow | Flow up annulus only, and |
| • Tubing Flow | Flow up drill pipe or tubing only. |

For the purposes of this project, the activity which leads to the scenario is not as important as the determination of flow rates and release characteristics associated with the scenario itself.

Figure 2.4 illustrates the geometry associated with a well blowout. The jet may be directed at any angle depending on the nature of the failure. All or part of the jet may be deflected by structures at the wellhead. Four specific cases (as depicted in Figure 2.4) were considered for this project:

- | | |
|----------------|-------------------------------------|
| • Downwind Jet | Horizontal jet pointing downwind, |
| • Vertical Jet | Vertical jet, |
| • Upwind Jet | Horizontal jet pointing upwind, and |
| • Cloud | Cloud (jet has lost momentum). |

Figure 2.4, for the purposes of illustration, shows the gas being released through a valve. A valve will usually be required to divert the vertical well flow to a non vertical release. Vertical releases, however, do not require the presence of a valve and can also occur from tubing and casing releases.

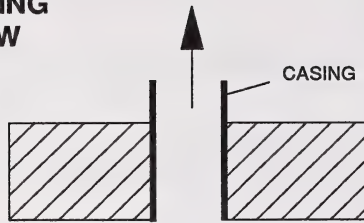
A horizontal jet pointing in the crosswind direction was not considered in this evaluation. The downwind and upwind jet were selected to be representative of the two extreme release angles (with respect to the wind direction) in the horizontal plane.

A minimum release height of one metre above the ground is taken as typical.

2.1.2 Pipeline Rupture

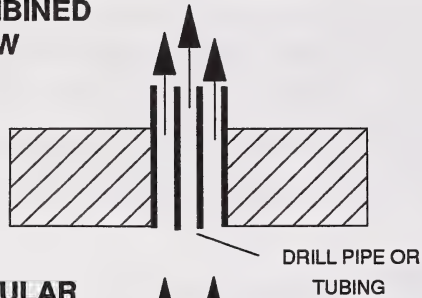
Sour gas pipelines are usually divided into a series of segments separated by emergency shut down (ESD) valves. In the event of a pipeline rupture, the ESD valves react to the pressure drop and isolate the ruptured segment from the rest of the system. Surface and/or subsurface ESD valves can also be placed at the wellhead. The purpose of the ESD valves is to limit the volume of sour gas which would be released to the atmosphere in the event of a failure. With the presence of ESD valves, the emission rate is characterized by a high initial flow rate which decreases with time as the pipeline is depressurized.

CASING FLOW



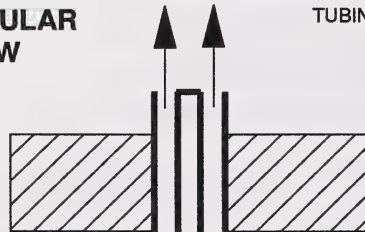
TRIPPING (U,S)
LOGGING (U)
CASING (U)
PERFORATING (U)

COMBINED FLOW



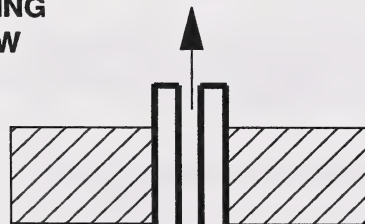
DRILLING (U)
TRIPPING (U,S)
CORING (U)
TESTING (U)
CASING (U)
PERFORATING (U)
STIMULATING (U,S)

ANNULAR FLOW



DRILLING (U)
TRIPPING (U,S)
CORING (U)
CASING (U)
STIMULATING (U,S)

TUBING FLOW



DRILLING (U)
TRIPPING (U,S)
CORING (U)
TESTING (U)
CASING (U)
PERFORATING (U)
STIMULATING (U,S)
PRODUCTION (S)

(U = UNSTIMULATED WELL)
(S = STIMULATED WELL)

FIGURE 2.3

Possible Well Flow Scenarios and Associated Activities.

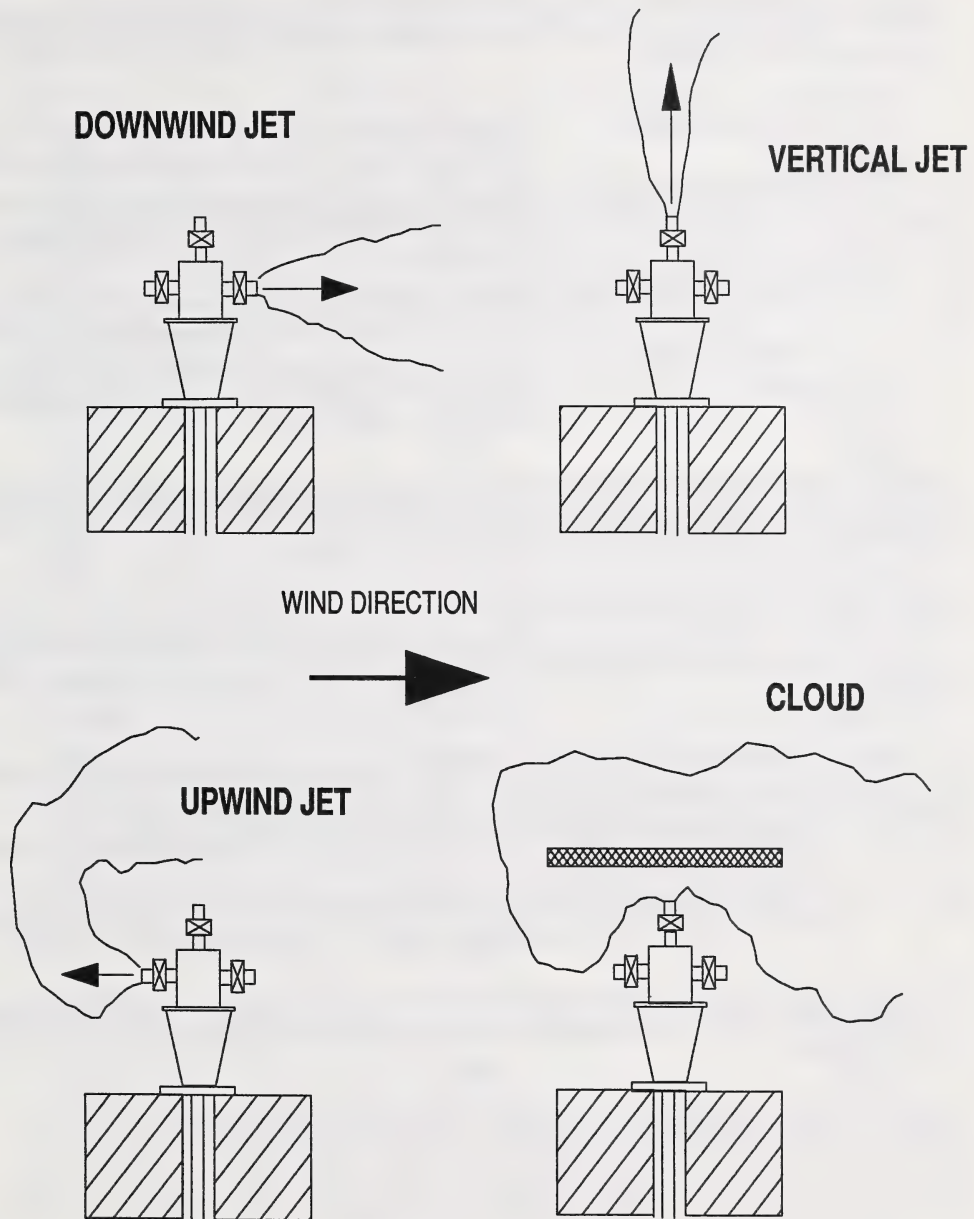


FIGURE 2.4
Possible Well Release Geometries.

Figure 2.5 illustrates typical valve and rupture configurations and the associated segments which would be depleted. These different depletion scenarios will affect the volume and release rate of the sour gas:

- | | |
|-------------------------|---|
| • End Pipe Rupture | Rupture adjacent to an ESD valve, all ESD valves operate as designed. One pipeline segment is depleted. |
| • ESD Valve Failure | Rupture at an ESD valve which fails, all other ESD valves operate as designed. Two pipeline segments are depleted. |
| • Center Pipe Rupture | Rupture between two ESD valves, all ESD valves operate as designed. One pipeline segment is depleted. |
| • Decay to Steady State | Rupture in segment next to wellhead, well ESD valve fails, and all other ESD valves operate as designed (An end rupture is depicted). |

The last scenario will be characterized by a transient release which will decay to the steady state flow driven by the formation pressure through the well. The other scenarios will be characterized by transient releases which will decay to zero.

Since there is a delay between the time of the rupture and time when the ESD valves are fully closed, the amount of sour gas released to the atmosphere will exceed the amount contained within the isolated segment of the line. This delay time is the summation of the following:

- Time for the pressure wave to travel from the rupture point to the ESD valve pressure sensor,
- Time for the pressure sensor to react to the pressure drop and initiate the closing of the ESD valve, and
- Time for the valve to fully close and completely isolate the ruptured segment from the rest of the gas gathering system.

The delay time of the system will depend on factors such as the length, diameter and operating conditions of the pipeline segment under consideration and the design and selection of ESD valve hardware.

END PIPE RUPTURE

ESD VALVE
OPERATES

ESD VALVE
OPERATES

ESD VALVE
OPERATES

ESD VALVE FAILURE

ESD VALVE
OPERATES

ESD VALVE
FAILS

ESD VALVE
OPERATES

CENTRE PIPE RUPTURE

ESD VALVE
OPERATES

ESD VALVE
OPERATES

ESD VALVE
OPERATES

DECAY TO STEADY STATE

ESD VALVE
FAILS

ESD VALVE
OPERATES

ESD VALVE
OPERATES

FIGURE 2.5

Possible Pipeline Rupture Scenarios.

As with a well blowout, the geometry associated with a pipeline rupture will determine the initial behavior of the sour gas in the atmosphere. Ruptures can occur above ground if they are located near an ESD valve or below ground. Pipeline ruptures can be caused by external or internal corrosion, metallurgical defects or mechanical (third-party) damage. The release geometries (as illustrated in Figure 2.6) can be broadly categorized as:

- Long Rupture (above or below ground)

A section of pipe is removed leading to two sources of gas, each being vented from an opening whose cross sectional area is equal to the cross sectional area of the pipe. Two opposing jets could result from such a configuration. For above ground ruptures, the orientation of these jets could range from horizontal to vertical. For below ground ruptures, the overburden is displaced within a few seconds and the two jets would be coming out of the ground at a small angle from the horizontal after being deflected by the walls of the crater created by the rupture.

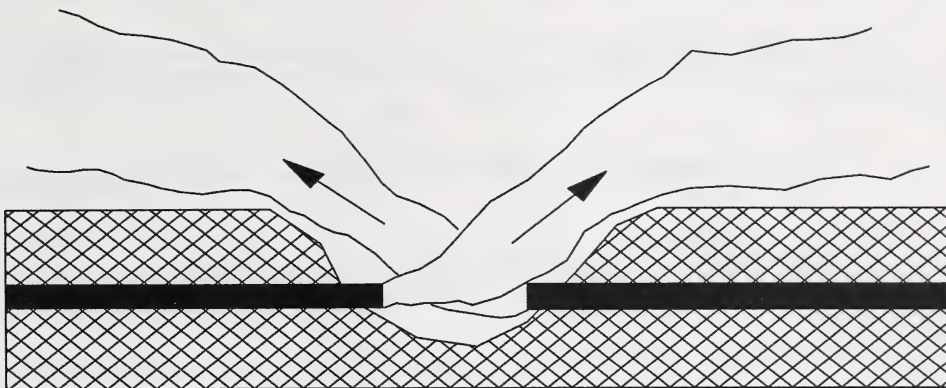
- Short Rupture (above or below ground)

A short rupture or split can occur on the top, bottom or side of the pipe. For top ruptures, a single, vertically oriented jet is expected. For bottom ruptures, the jet will be deflected by the crater formed during the rupture. This crater will result in a ground-level cloud release with negligible vertical momentum. For side ruptures, a single horizontal jet will result for above ground ruptures; for below ground ruptures the jet will be directed at a small angle from the horizontal or will act as a ground-level release. The cross sectional area of the opening will be typically equal to the cross sectional area of the pipe.

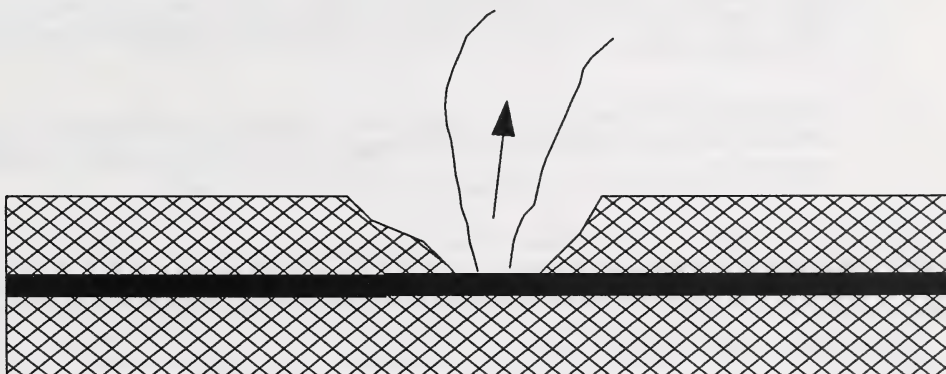
- Leak (above or below ground)

Leaks can develop from localized corrosion and are typically pinholes. For below ground failures, the overburden may not be disturbed appreciably allowing the gas to diffuse through the ground and emerge as a ground-level release with negligible momentum.

LONG RUPTURE



SHORT RUPTURE



LEAK

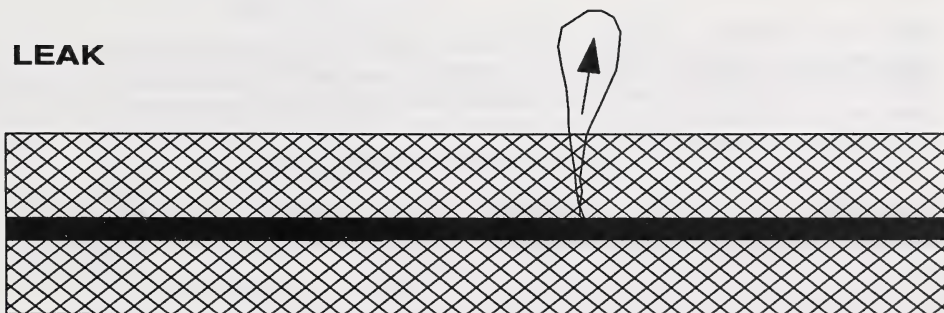


FIGURE 2.6

Possible Pipeline Release Geometries.

2.2 Meteorology

The meteorology during an uncontrolled release is perhaps the most important parameter which determines the extent of an exposure zone. The meteorological parameters of importance are:

- Wind Direction Controls the direction of the plume which determines the plume impact zone.
- Wind Speed Wind speed directly controls the along wind spread of the sour gas plume and indirectly affects the rise of plume and the turbulence in the atmosphere.
- Turbulence The level of turbulence in the atmosphere controls the dilution of the plume. Turbulence can be generated by wind shear or heat convection.
- Mixing Height Elevated temperature inversions can act as a lid restricting the vertical movement of a gas plume. This restriction can reduce the dilution capacity of the atmosphere.
- Temperature The buoyant rise of a gas plume depends on the difference in density between the gas and the atmosphere. Atmospheric density depends on ambient temperature.

All of these parameters can be measured directly in the atmosphere. Wind direction, wind speed and temperature are measured on a routine basis at meteorological stations operated by the Atmospheric Environment Service (AES). These data are typically available on an hourly basis. The AES wind observations represent a single one-minute averaging period for each hour. For dispersion modelling purposes, a true one-hour average would be preferable.

AES does not monitor turbulence and mixing heights on a routine basis because they are not perceived as being important for synoptic weather forecasts (which are primarily undertaken for transportation sector and public interests). These parameters, therefore, may have to be estimated from what routine measurements are available and from our understanding of the behavior of the planetary boundary layer.

2.2.1 Planetary Boundary Layer

The "Planetary Boundary Layer" refers to the lowest level of the atmosphere whose properties are directly influenced by surface heating and wind shear. The layer of the atmosphere above the boundary layer is referred to as the free atmosphere. The depth of the planetary boundary layer (PBL) over land typically ranges from 100 to 300 m at night to 1000 to 2000 m during the day. The PBL can be broadly classified as convective, neutral and stable according to the surface heat flux (the rate of energy transfer from the ground to the air).

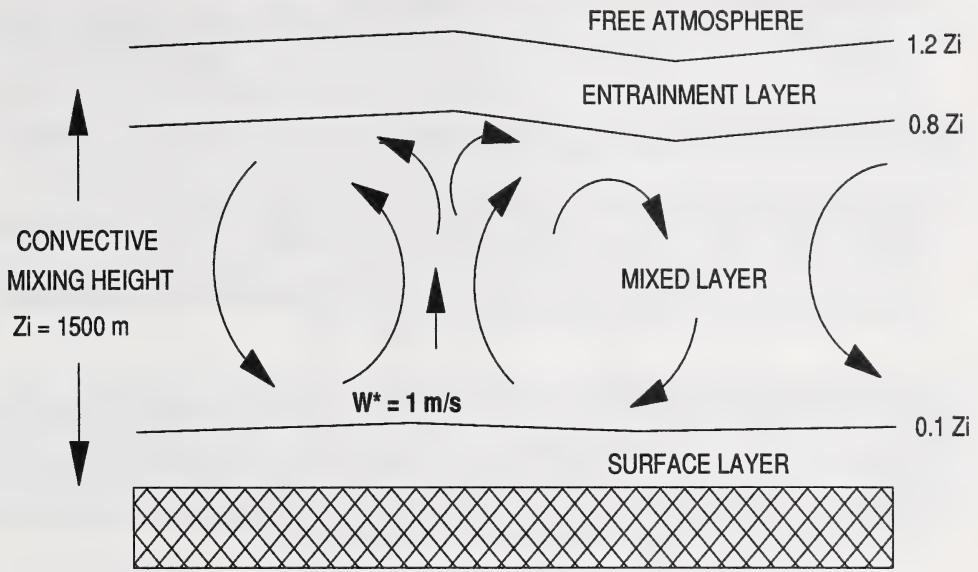


FIGURE 2.7

Structure of the Convective Planetary Boundary Layer.

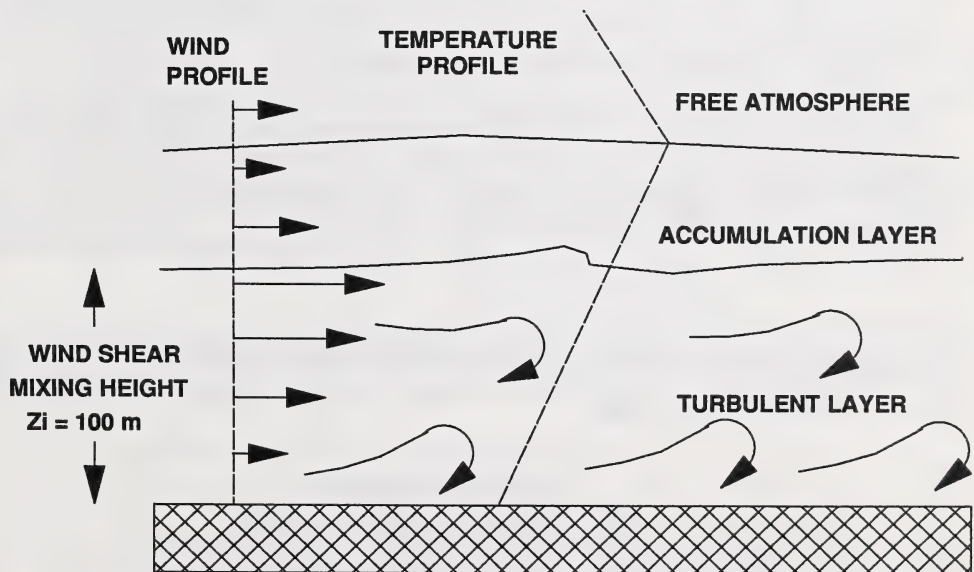


FIGURE 2.8

Structure of the Stable Planetary Boundary Layer.

Periods when the surface heat flux is positive (typically daytime conditions) are referred to as convective or unstable. The depth of the convective PBL typically deepens during the day, ranging from a few hundred metres just after sunrise to 1000 to 2000 m by mid-afternoon. The convective boundary layer is well mixed due to large eddies which are generated by the heating of the earth's surface. These large eddies result in the rapid and uniform mixing of pollutants in the vertical (Figure 2.7).

At sunset, the PBL turbulence levels decrease when the surface heat flux becomes negative (typically night time conditions). During these stable conditions, pollutants released from surface sources tend to remain near the ground and pollutants released from elevated sources tend to remain aloft. The depth of the mixed layer under stable conditions is driven by wind shear and typically ranges from 100 to 200 m (Figure 2.8).

Neutral conditions occur when turbulence is neither enhanced (as in unstable conditions) nor suppressed (as in stable conditions). Neutral conditions can occur during transition periods (unstable to stable and vice-versa) or under high wind speed conditions when mechanical shear forces dominate turbulence. During these high wind speed neutral conditions, plume rise is minimal and the plume can be thought of as horizontally oriented cone that increases in diameter as the plume moves downwind.

2.2.2 Unstable Conditions

Strong solar heating produces large scale, highly turbulent, convective motions in the form of updrafts and downdrafts as depicted in Figure 2.7. The convective mixing layer is divided into three layers. The surface layer is where wind shear is important. The mixed layer is relatively uniform due to vigorous mixing by convective activity. The entrainment layer is the interface between the PBL and the free atmosphere.

These convective motions have dimensions which are proportional to the mixing height (Z_i) and updraft velocities which are typically equal to the convective velocity scale (W^*) (Deardorff, 1972). Typical mid-afternoon values for W^* range from 1 to 2 m/s. The terms Z_i and W^* have been used successfully to classify turbulence under convective conditions for laboratory experiments (Willis and Deardorff, 1974) and for full scale field simulations (Kaimal *et al.* 1976).

Turbulence can also be generated from wind shear (mechanical mixing processes). The ratio Z_i/L indicates the relative importance of convective and wind shear generated turbulence (where L is the Monin-Obukhov length). Qualitative interpretations of this ratio are as follows (e.g., Briggs 1986):

- $Z_i/L > 100$ Very unstable conditions.
- $20 < Z_i/L < 100$ Moderately unstable conditions.
- $10 < Z_i/L < 20$ Slightly unstable conditions.
- $Z_i/L < 10$ Wind shear starts to dominate.

The Monin-Obukhov length, L , is defined by the relationship given later in the report (Equation 3.15) and can be thought of as the depth of the mechanically mixed surface layer (Hanna *et al.* 1982). The Monin-Obukhov length is independent of height in the surface

layer and is a function of the surface friction velocity (U^*). The friction velocity is the velocity scale most directly associated with turbulent motions in the surface layer (lowest level of the PBL).

For unstable conditions, L assumes a negative value since the surface heat flux is positive. During periods of strong convection, $|L|$ can be as small as 10 m and during periods of high wind speeds with small positive heat flux values, $|L|$ can typically reach large values (100 m). For pure mechanically generated turbulence, the value of $|L|$ approaches infinity.

2.2.3 Stable Conditions

The turbulent mixing layer associated with stable conditions is much thinner than that associated with unstable conditions (Figure 2.8). The accumulation layer in the figure refers to the accumulation of air which is colder than that of the free atmosphere due to katabatic effects (terrain induced cold air drainage). Since turbulence reaches a minimum at the top of the mixing layer, pollutants emitted from elevated sources in the PBL can also "accumulate" in this region (Wetzel, 1982).

Since turbulence in the stable boundary layer is generated by wind shear, the Monin-Obukhov length (L) and the surface friction velocity (U^*) are the important parameters. Stable conditions are associated with negative values of the heat flux, and as a consequence, positive values of L . Under light wind speed conditions, L can be as small as 10 m. Reported values for L are seldom less than 10 m since the lowest few metres of the atmosphere tend to be nearly neutral under nearly all conditions. As the wind speed increases, values of L also increase.

Under stable conditions the ratio Z_i/L indicates the relative importance of suppression of mechanical turbulence by temperature stratification. Qualitative interpretations of this ratio are as follows (e.g., Panofsky and Dutton, 1984):

- | | |
|-----------------------------|--|
| • Z_i/L slightly positive | Mechanical turbulence slightly damped by temperature stratification. |
| • Z_i/L strongly positive | Mechanical turbulence severely damped by temperature stratification. |

A number of definitions have been proposed for the depth of the turbulent layer (Z_i). These include the:

- Height of the low-level wind speed maximum,
- Height to which significant cooling extends,
- Top of the surface temperature inversion, and
- Height of the lowest discontinuity in the temperature profile.

The intent of the above definitions of the mixing layer height is to define the region where turbulent diffusion takes place. The above definitions require information on the vertical profiles of wind speed and temperature. Wetzel (1982) evaluated the different definitions and found that Z_i could be best defined by the lower of the level where the wind speed is a maximum or the level to which significant cooling occurs.

2.2.4 Neutral Conditions

The occurrence of the classic "neutral" atmosphere associated with a near zero surface heat flux is often thought of as being relatively rare (Panofsky and Dutton, 1984; Briggs, 1986; Wyngaard, 1986). For practical dispersion modelling purposes, however, a well mixed atmosphere whose turbulence is primarily generated by wind shear can be assumed to be neutral. For example, during positive heat flux (unstable) conditions, if the wind speed (U_{REF}) is large compared to the convective velocity scale (W^*) then wind shear generated turbulence can be assumed to be more important than convective turbulence (Weil and Brower, 1984). In this case, neutral conditions can be assumed. Similarly, during negative heat flux (stable) conditions, if the Monin-Obukhov length (L) is large then the boundary layer can be assumed to be neutral (OME, 1986).

Under neutral conditions, the height of the turbulent layer (Z_i) will also depend on the vertical temperature profile. The height of the neutral turbulent layer is often defined by the height of the overlying temperature inversion layer (Wyngaard, 1986).

2.2.5 Atmospheric Boundary Layer Parameters

In summary the following parameters can be used to characterize the turbulent behavior of the PBL:

- Unstable conditions

Convective mixing depth (Z_i)
Convective velocity scale (W^*)
Friction velocity (U^*)

- Stable and neutral conditions

Wind shear mixing depth (Z_i)
Friction velocity (U^*)

A meteorological data processor (often called a preprocessor) can be used to determine these parameters from standard meteorological observations. Section 3 discusses the development of a preprocessor which can be used to estimate the above parameters from routine AES meteorological observations.

2.3 Consequences

The chemical compounds of primary concern in sour gas are H_2S for the unignited release case and SO_2 (which results from the combustion of H_2S) for the ignited release case. Physiological responses to these components are dependent on the magnitude of the concentration, the duration of the exposure period and individual susceptibility. Discussion of physiological responses to H_2S are important to describe the adverse effects and thus the consequences. The approach presented in this study is sufficiently flexible that different criteria can be adopted for different needs.

If a sour gas well blowout were to occur, the toxic effect of H_2S would depend on the length of time people would be exposed to the toxic gas. This exposure time would strongly depend on the delay time for ignition of the sour gas release from a well blowout or the time to deplete a ruptured pipeline segment.

Observations made in animal experiments and some documented cases of accidental human exposure to toxic gas show a systematic relationship between the likelihood of adverse effects of toxic gas and concentration level and exposure time. This relationship is dependent on the toxic gas (e.g. H_2S) and on the nature of the adverse effect (e.g. fatality). The parameters necessary to determine precisely this relationship are necessary inputs to the model.

Variation in Toxic Gas Concentration

Peak concentrations may be several times the average concentration due to the natural turbulent motions of air in the atmosphere. Toxic loads based on average concentrations are not adequate to model adverse effects since the periods of peak concentrations would be severely understated.

The model incorporates a current model for concentration variability in its treatment of detrimental effects. Because human susceptibility is modelled as toxic load dependent, the GASCON2 model is capable of handling the peak periods in toxic gas concentration and the exposure time.

Population Density

The potential number of people that can be adversely affected by an accidental sour gas release is dependent on the population density (people per square kilometer) in the exposure zone around a sour gas facility.

Returning to the specific hazard with which this work is concerned, namely, uncontrolled releases of sour gas from well blowouts and pipeline ruptures, it is necessary to define precisely the scope of the consequences to be determined.

Figure 2.9 shows the general elements which make up a risk assessment. Foremost in the scheme is the identification of an uncontrolled sour gas release event. For the purposes of this work, an uncontrolled sour gas release event is defined as the combination of sour gas source and meteorological conditions which completely determine the influence of the sour gas release on the surroundings. The two fundamental portions of a risk assessment are the frequency analysis and the consequence analysis.

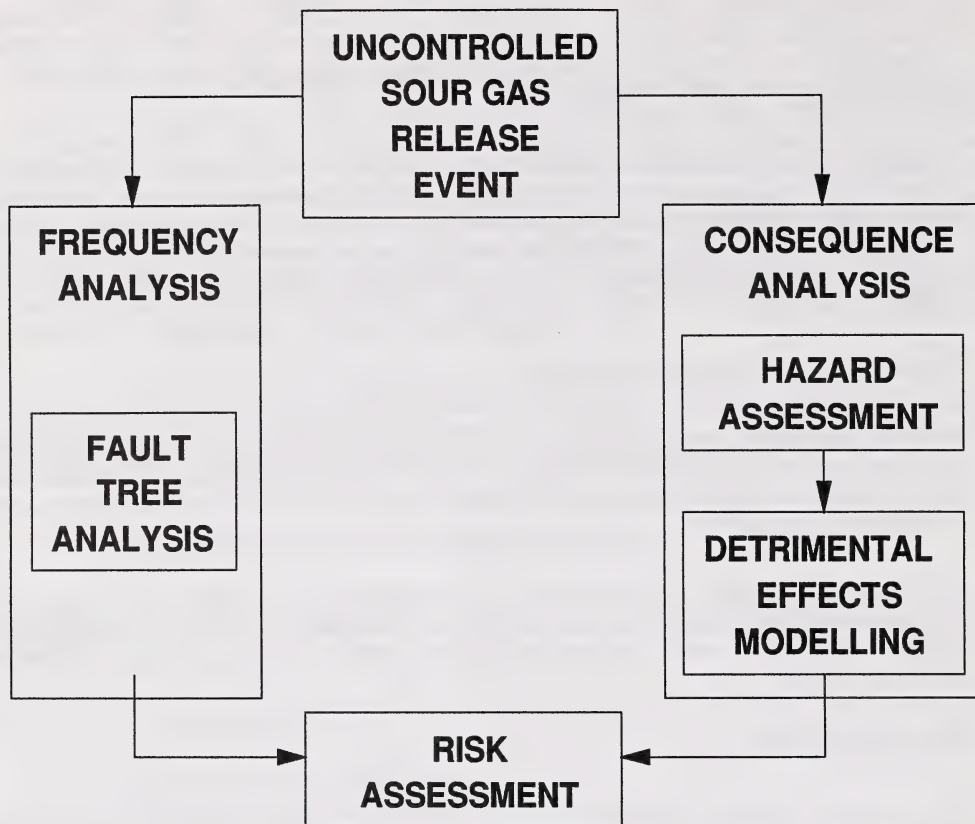


FIGURE 2.9

General Risk Assessment Elements.

The frequency analysis estimates the frequency of occurrence of a release event; in other words, how likely is it that a specific release event could occur? The main tool of the frequency analysis is a technique called fault tree analysis, which is described in detail in Volume 6 (Alp *et al.* 1990).

The consequence analysis in Figure 2.9 estimates the detrimental effect of an uncontrolled sour gas release. Hazard assessment is used to estimate the extent of influence of the release and effects modelling is used to estimate the detrimental effect of the release. The detrimental effect of concern for this risk assessment of uncontrolled sour gas releases is lethality to humans; that is, the potential for human fatality due to exposure to, and inhalation of, the toxic sour gas component (H_2S). The justification for considering lethal effects to humans in this risk assessment is given in Section 4.6, along with a discussion of the difficulties associated with considering sub-lethal effects.

The fluctuating load and probit module provides the necessary link between the extent of influence of a sour gas release and the detrimental effect of this influence. This is accomplished by relating the H_2S concentration at a given downwind location to the probability that the dose of H_2S a person would receive is lethal.

2.3.1 Individual Risk and Societal Risk

In Figure 2.1 detrimental effects are determined in the "fluctuating toxic load" and "probability of lethality modules". These modules accounts for two very important factors in the determination of the detrimental effects to people due to an accidental sour gas release of toxic gas. The first factor is the variation in toxic gas concentration ("fluctuating load") due to the natural turbulence in the atmosphere. The second factor is the human susceptibility to toxic gas exposure ("probit analysis"). Together these two factors give an estimate of the likelihood that people exposed to sour gas during an accidental release would be adversely affected. The GASCON2 model also estimates "individual risk" and "societal risk".

As used in this study, individual risk is the likelihood that a person downwind of an uncontrolled sour gas release will receive a lethal exposure of H_2S . This probability will vary from one downwind location to another, since the H_2S concentrations are location dependent. In this work, the individual risk is reported for a specific release event, whose frequency of occurrence is known from the frequency analysis portion of the risk assessment; individual risk is not summed over all possible release events. Rather, the individual risk at several downwind locations assume that the given release event occurs. A wide range of release events are considered.

Societal risk is an estimate of the potential number of human fatalities which could result from an uncontrolled sour gas release. This may be viewed as the sum of the individual risks of all the people in the area exposed to the sour gas release. In this work, societal risk is reported for a specific release event. Societal risk for a given release event is reported separately from the frequency of occurrence of that release event.

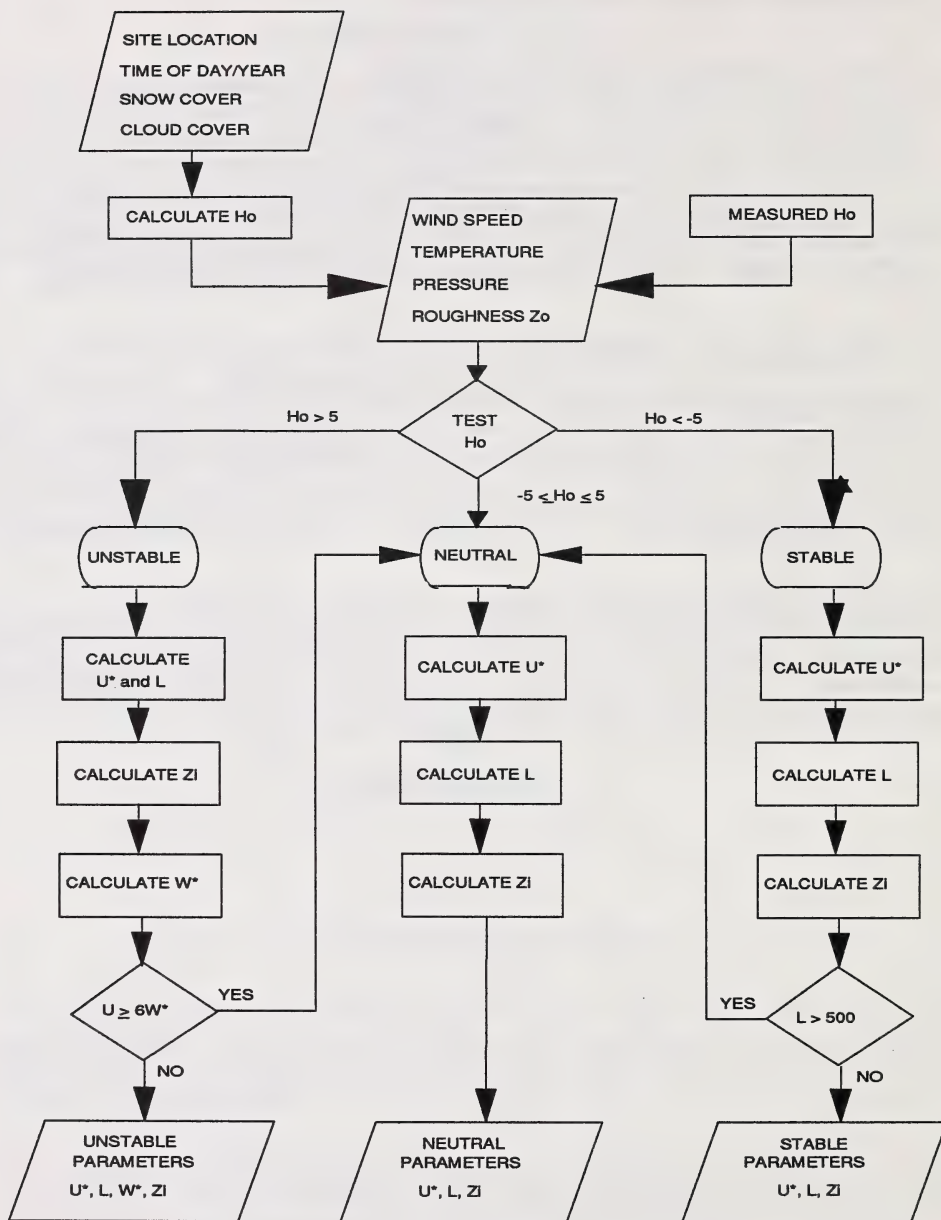


FIGURE 3.1

Atmospheric Stability Determination Flow Chart.

3 METEOROLOGICAL DATA PROCESSOR

This section of the report presents a meteorological data processor which can be used to provide meteorological data for the dispersion modelling system. The meteorological data processor (or preprocessor) estimates atmospheric stability and the associated boundary layer parameters from routine meteorological observations. Since dispersion models are sensitive to meteorological assumptions, better input data through the use of a well designed meteorological preprocessor should result in improved model predictions (van Ulden and Holtslag, 1985).

The preprocessor described can be applied to several years of routine Atmospheric Environment Service (AES) data to either estimate the atmospheric boundary layer parameters on an hour-by-hour basis or to estimate the statistics associated with the predicted parameters. For the purposes of illustration, the preprocessor was applied to five years of routine meteorological data from Calgary International Airport and sample results are also presented in this section. The results of the preprocessor output were then compared to traditional methods of estimating atmospheric stability.

3.1 Preprocessor Approach

Figure 3.1 depicts the flow chart used to determine stability and the associated PBL parameters. The surface heat flux (H_o) has to be estimated first. Once H_o is known, the other PBL parameters can be estimated using site-specific surface parameters and meteorological observations.

Meteorological observations are available from the AES Digital Archive on an hourly basis. These data allow the stability class and the PBL parameters to be determined on an hourly basis. The required routine observations are:

- Surface pressure (P_{AO})
- Surface ambient temperature (T_{AO})
- Fraction cloud cover (C)
- Snowing indicator
- Snow depth
- Wind speed (U_{REF})
- Wind direction.

All of the above, except snow depth, are available on an hourly basis from the AES in HLY01 record format (AES, 1983). Snow depth information is available on a daily basis in DLY04 record format (AES, 1983).

3.1.1 Surface Heat Flux

The surface heat flux is transfer of energy from the ground to the atmosphere which is in contact with the ground. During sunny day-time conditions, the energy transfer is positive (from the ground to the atmosphere) and during night-time conditions the energy transfer is negative (from the atmosphere to the ground). The heat flux at the earth's surface may be assumed to be proportional to the net solar radiation with a correction factor for long wave radiation loss from the ground (Scire *et al.* 1984):

$$H_o = \tilde{\alpha}\tilde{R} + H_L \quad (3.1)$$

where: H_o = surface heat flux (W/m^2)
 $\tilde{\alpha}$ = reduction factor due to surface reflectivity
 = 0.00 if there is snow cover
 = 0.35 otherwise
 $\tilde{R}$ = incoming solar radiation (W/m^2)
 H_L = heat flux in the absence of solar incoming radiation (W/m^2).

The incoming solar radiation can be expressed as:

$$\begin{aligned} \tilde{R} &= 950 \tilde{\beta} \sin \phi \text{ between sunrise and sunset and} \\ \tilde{R} &= 0 \text{ between sunset and sunrise} \end{aligned} \quad (3.2)$$

where: $\tilde{\beta}$ = reduction factor due to cloud cover
 = $1 - 0.001(9.54C - 0.0807C^2 - 0.000473C^3 + 0.0000110C^4)$
 ϕ = solar elevation angle above the horizon
 C = cloud cover in percent.

The cloud cover reduction factor ($\tilde{\beta}$) was determined from a curve fit to data reported by Scire *et al.* (1984) and Maul (1980).

The heat flux in the absence of solar incoming radiation from the surface can be estimated from (Scire *et al.* 1984):

$$H_L = -0.24(112.5 - C) \quad (3.3)$$

Sunrise and sunset times and the solar elevation angle can be estimated from the latitude and longitude of the site, the time zone standard longitude, the time of the day and the time of the year (Table 3.1). Hourly values of the snow cover can be estimated from the hourly snowing indicator and the daily snow depth values (Table 3.2).

Equation 3.1 ignores the latent and soil heat flux terms. The latent heat flux term decreases the amount of sensible heat which can be transferred from the surface to the air due to evaporation of surface moisture. The latent heat flux term can be significant for moist surfaces and insignificant (~ 0) for dry surfaces. The soil heat flux accounts for the transfer of energy into the ground. This term is typically much smaller (less than 10% of $\tilde{R}$) than the other heat flux terms. The exclusion of the latent and soil heat flux terms was not viewed as contributing to significant errors in the estimation of H_o in Alberta.

Table 3.1
Calculation of Solar Related Parameters.

Solar Elevation Angle $\tilde{\phi}$

- (1) The sine of the solar elevation angle is given by:

$$\sin \tilde{\phi} = \cos \tilde{\delta} \cos \tilde{\tau} \cos L_T + \sin \tilde{\delta} \sin L_T \quad (3.4)$$

where: L_T = latitude of site (e.g. 51° for Calgary) (degrees)
 $\tilde{\tau}$ = hour angle (radian)
 $\tilde{\delta}$ = solar declination (radian)

- (2) The hour angle is given by:

$$\tilde{\tau} = \frac{\pi}{12} \left[t - 12 + \frac{(L_{ST} - L_O)}{15} \right] \quad (3.5)$$

where L_{ST} = time zone standard longitude (e.g. 105° for MST) (degrees)
 L_O = longitude of site (e.g. 114° for Calgary) (degrees)

- (3) The solar declination is expressed as:

$$\tilde{\delta} = \tan^{-1} \left[0.4348 \sin \left(\frac{\pi(D - 78)}{180} \right) \right] \quad (3.6)$$

where D = Julian day of the year (1 to 365)

Sunrise and Sunset Times

- (1) The sunrise (t_{RISE}) and sunset (t_{SET}) times are:

$$t_{RISE} = t_N - \frac{12}{\pi} \cos^{-1}(-\tan \tilde{\delta} \tan L_T) \quad (3.7)$$

$$t_{SET} = t_N + \frac{12}{\pi} \cos^{-1}(-\tan \tilde{\delta} \tan L_T) \quad (3.8)$$

- (2) where t_N = local standard noon time in decimal hours given by:

$$t_N = 12 - \left(\frac{L_{ST} - L_O}{15} \right) \quad (3.9)$$

The estimation of the above solar related parameters ignores the "Equation of Time" correction factor (Abell, 1969). This correction factor is a function of time of year and can amount to ± 15 minutes correction in the above calculated sunset and sunrise times. This correction factor is not viewed as being significant for the purposes of estimating H_O .

Table 3.2

The Determination of Hourly Snow Cover.

The Atmospheric Environment Service (AES) Digital Archive contains information as to whether it is snowing during a given hour and the depth of snow on the ground for each day. With these data, it is possible to construct an algorithm for making a reasonable decision about hourly snow cover. Based on the daily observations of snow on the ground for a given day and for the previous day, four possibilities exist:

- | | |
|-----|---|
| (1) | The given day has snow on the ground, but the previous day did not. |
| (2) | The given day has snow on the ground, and so did the previous day. |
| (3) | The given day has no snow on the ground, but the previous day did. |
| (4) | The given day has no snow on the ground, nor did the previous day. |

Cases (2) and (4) are easiest to handle. If two consecutive days have snow on the ground, then it is reasonable to assume that there is snow cover for every hour of the second day. On the other hand, if two consecutive days have no snow on the ground then it may be assumed that there is no snow cover for every hour of the second day.

Case (1) requires additional information to assess hourly snow cover. By referring to the hourly meteorological records it is possible to find the hour during the given day when it first begins to snow. Before that time, no snow cover is assumed for every hour on the given day; after that time, snow cover is assumed for every hour on the given day.

Case (3) also requires reference to the hourly records. At some time on the given day the snow on the ground must melt, and this time is assumed to be the hour on the given day when the maximum ambient temperature occurs. Before that hour, snow cover is assumed for every hour on the given day.

3.1.2 Convective Mixing Layer Height

Between sunset and sunrise, the convective mixing height is assumed to be zero. Between sunrise and sunset, if the vertical temperature gradient is not known at the time of the minimum temperature then the convective mixing height can be estimated from the simplified relationship (Panofsky and Dutton, 1984):

$$Z_i = \frac{2}{C_{PA}\rho_{AO}[T_{AO}(t) - T_{AO}(\min)]} \int_{t_o}^t H_o dt \quad (3.10)$$

Alternatively, if the vertical temperature gradient is known at the time of the minimum temperature then:

$$Z_i = \left(\frac{2}{C_{PA}\rho_{AO}(\gamma_D - \gamma)} \int_{t_o}^t H_o dt \right)^{1/2} \quad (3.11)$$

where:

- Z_i = convective mixing height (m)
- H_o = surface heat flux (W/m^2)
- C_{PA} = specific heat of air at constant pressure (1005 J/(kg K))
- ρ_{AO} = ambient air density (kg/m^3)
- $T_{AO}(t)$ = ambient surface temperature at time t (K)
- $T_{AO}(\min)$ = minimum ambient surface temperature after sunrise (K)
- γ_D = dry adiabatic lapse rate (0.0098 K/m)
- γ = minimum lapse rate after sunrise (K/m) ($\gamma = -dT/dz$).

This relationship indicates that Z_i at time t depends on the square root of the surface heat flux prior to time t and that Z_i is expected to grow linearly with time in the early morning hours. As the day progresses, Z_i will continue to grow at an ever decreasing rate.

In the estimation of hourly values of Z_i the following rules specified by Benkley and Schulman (1979) are applied:

- $Z_i = 0.0$ between sunrise and the time of the minimum temperature which normally occurs after sunrise. If the temperature continues to drop throughout the day then $Z_i = 0.0$ for that day.
- Transient decreases of Z_i during the day are not allowed.
- The maximum value of Z_i is associated with the maximum temperature during the day ($T_{AO}(\max)$). Z_i is not allowed to increase between the time corresponding to $T_{AO}(\max)$ and sunset.
- Transition from daytime $Z_i(\max)$ to nighttime $Z_i = 0.0$ occurs when $T_{AO} = T_{AO}(\max) - 0.25 [(T_{AO}(\max) - T_{AO}(\min))]$.

The above estimations for Z_i ignore the fact that energy can also be added to the mixed layer from the sides and the top (entrainment from the stable air aloft) and that horizontal transport (advection) may cause a local change in Z_i .

Notwithstanding the previous discussion, a lower limit of 50 m for the convective mixing layer height Z_i based on observations has been selected for mid-day conditions (Holzworth, 1967; Pasquill and Smith, 1983).

3.1.3 Convective PBL Parameters

Convective or unstable conditions are assumed to occur for surface heat fluxes H_o greater than 5 W/m^2 . The surface friction velocity (U^*) can be estimated from the log-linear wind profile (Panofsky and Dutton, 1984):

$$U^* = \frac{k U_{REF}}{\ln\left(\frac{Z_{REF}}{Z_o}\right) - \Psi\left(\frac{Z_{REF}}{L}\right)} \quad (3.12)$$

where:

- k = von Karman constant (~ 0.4)
- U_{REF} = wind speed at anemometer height (m/s)
- Z_{REF} = anemometer height (m)
- Z_o = surface roughness length (m)
- L = Monin-Obukhov length (m).

The stability parameter for unstable conditions is given by:

$$\Psi\left(\frac{Z_{REF}}{L}\right) = 2 \ln\left(\frac{1+\bar{q}}{2}\right) + \ln\left(\frac{1+\bar{q}^2}{2}\right) - 2 \tan^{-1}(\bar{q}) + \frac{\pi}{2} \quad (3.13)$$

where:

$$\bar{q} = \left(1 - 15 \frac{Z_{REF}}{L}\right)^{1/4} \quad (3.14)$$

The Monin-Obukhov length (L) is defined from:

$$L = -\frac{\rho_{AO} C_{PA} \bar{T}_A U^{*3}}{k g H_o} \quad (3.15)$$

Using the ideal gas law, the above equation may be rewritten as:

$$L = -\frac{P_{AO} C_{PA} \bar{T}_A U^{*3}}{g k H_O R_A T_{AO}} \quad (3.16)$$

where $\bar{T}_A$ is the average temperature in the convective boundary layer and is given by:

$$\bar{T}_A = 0.5(2T_{AO} - \gamma_D Z_i) \quad (3.17)$$

and:

$$\begin{aligned} \gamma_D &= \text{dry adiabatic lapse rate (0.0098 K/m)} \\ R_A &= \text{gas constant for air (287 J/(kg K))} \\ P_A &= \text{surface atmospheric pressure (Pa)} \\ T_{AO} &= \text{ambient surface temperature (K).} \end{aligned}$$

The estimation of L and U^* is iterative in nature and can be solved by the approach given in Table 3.3. Once these parameters have been estimated, the convective velocity scale can be readily calculated from:

$$W^* = \left(\frac{g H_O Z_i}{\rho_{AO} C_{PA} \bar{T}_A} \right)^{1/3} = U^* \left(-\frac{Z_i}{kL} \right)^{1/3} \quad (3.18)$$

If the wind speed (U_{REF}) equals or exceeds $6 W^*$, then wind shear is assumed to be more important than convective eddies and the boundary layer is assumed to be neutral. Z_i is calculated from Section 3.1.2 or input by the user. The minimum value of Z_i is 50 m.

Finally, if the PBL is classified as unstable, the ratio of $Z_i / -L$ must be greater than 2.0. If the ratio is less than 2.0, either Z_i or L are adjusted as follows, depending on H_O :

$$L = -0.5Z_i + .01 \text{ if } H_O < 20$$

$$Z_i = -2L + .01 \text{ if } H_O \geq 20$$

Table 3.3

Solution for L and U^* for Unstable Conditions.

The calculation of L and U^* is iterative in nature and can be solved through the adoption of the following procedure:

- (1) Assume a value for the stability function $\Psi(Z_{REF}/L)$ of zero.
- (2) Calculate a value for the friction velocity U^* (Equation 3.12).
- (3) Calculate a value for the Monin-Obukhov length L (Equation 3.16).
- (4) Calculate a value for the term $\bar{q}$ (Equation 3.14).
- (5) Calculate a new value for the stability function $\Psi(Z_{REF}/L)$ (Equation 3.13).
- (6) Calculate a new value for the friction velocity U^* (Equation 3.12).
- (7) If the difference between the new value for U^* and the previous value for U^* is less than 0.1 percent proceed to Step (8). If the difference is greater than 0.1 percent then go back to Step (3).
- (8) The most recent value U^* is the selected value for U^* , this value is used to calculate a value for L .

3.1.4 Neutral PBL Parameters

Neutral conditions occur for surface heat fluxes (H_o) between -5 and +5 W/m². For surface heat flux near zero, the following adjustments are made to prevent L from approaching infinity:

$$H_o = 1 \quad \text{if} \quad 0 \leq H_o < 1$$

$$H_o = -1 \quad \text{if} \quad -1 < H_o < 0$$

The surface friction velocity can be estimated from the logarithmic wind profile for neutral conditions (Panofsky and Dutton, 1984):

$$U^* = \frac{k U_{REF}}{\ln\left(\frac{z_{REF}}{z_o}\right)} \quad (3.19)$$

The Monin-Obukhov length (L) may be then estimated from:

$$L = -\frac{\rho_{A0} C_{PA} T_{AO} U^{*3}}{k g H_o} \quad (3.20)$$

This compares to Equation 3.15 where the average temperature in the mixing layer ($\bar{T}_A$) is used for unstable conditions. For neutral conditions, the surface temperature (T_{AO}) is used since the mixing heights for neutral conditions tend to be less than those for unstable conditions.

The mixed layer height Z_i may be obtained from the expression (van Ulden and Holtslag, 1985):

$$Z_i = \frac{0.2 U^*}{f_c} \quad (3.21)$$

where: f_c = Coriolis parameter = $2\Omega \sin L_T$

Ω = Earth's rotation rate ($7.272 \cdot 10^{-5} \text{ s}^{-1}$)

For Calgary ($L_T = 51^\circ \text{N}$), the Coriolis parameter is $1.1 \cdot 10^{-4} \text{ s}^{-1}$.

3.1.5 Stable PBL Parameters

Stable atmospheric conditions are assumed to occur for surface heat fluxes H_o less than -5 W/m^2 . The surface friction velocity can be estimated from the log-linear wind profile (Panofsky and Dutton, 1984):

$$U^* = \frac{k U_{REF}}{\ln\left(\frac{Z_{REF}}{Z_o}\right) - \psi\left(\frac{Z_{REF}}{L}\right)} \quad (3.22)$$

For stable conditions:

$$\psi\left(\frac{Z_{REF}}{L}\right) = -4.7 \left(\frac{Z_{REF}}{L}\right) \quad (3.23)$$

The logarithmic wind profile relationship (Equation 3.22) can be used with the defining expression for the Monin-Obukhov length (Equation 3.20) to yield a cubic equation for U^* which may be solved iteratively for the largest real root. For the cases when no real root exists for U^* , the approach taken in Table 3.4 is adopted. This approach leads to a minimum value for U^* . Physically, a non-zero asymptotic value of U^* (for a given Z_{REF} , U_{REF} and Z_o) is justifiable in that a certain level of turbulence is always observed in a stable boundary layer (residual turbulence).

The approach given in Table 3.4 is less restrictive than other approaches which have been used to resolve the problem. For example, OME (1986) defines a minimum value for U_{REF} which is used in subsequent plume rise and concentration calculations. One minimum value for U_{REF} is 2.6 m/s (Venketram, 1980). The approach in Table 3.4 allows U_{REF} values less than 2.6 m/s to be used. An alternative approach uses a different vertical wind speed profile for large Z_{REF}/L ratios (e.g., Webb, 1970; Hicks, 1976; Lettau, 1979). Because the precise nature of this profile has yet to be established, the approach described in Table 3.4 was used.

The height of the stable mixing layer (Z_i) may be estimated from (Nieuwstadt, 1981):

$$Z_i = \frac{L}{3.8} \left(\sqrt{1 + 1.52 \frac{U^*}{L f_c}} - 1 \right) \quad (3.24)$$

In strongly stable conditions (small values of L), Equation 3.24 will predict values for Z_i which approach the Zilitinkevich (1972) expression for Z_i . In less stable atmospheres where neutral conditions are approached (larger values of L), Equation 3.24 will predict values for Z_i which approach the neutral value for Z_i (Equation 3.21). The minimum Z_i value predicted for stable conditions is 28 m for a wind speed (U_{REF}) of 1 m/s and a surface heat flux (H_o) of -27 W/m^2 (the most stable limits).

If the predicted value of L exceeds 500 m, then the boundary layer is assumed to be neutral.

Table 3.4
Solution for L and U^* for Stable Conditions.

In strongly stable conditions, no solutions for U^* and L exist when:

$$\frac{Z_{REF}}{L} > \frac{1}{2(4.7)} \ln \left(\frac{Z_{REF}}{Z_O} \right) \quad (3.25)$$

which is equivalent to:

$$U_{REF} < \frac{3}{k} \left[-\frac{4.7 Z_{REF} g k H_O R_A}{4 C_{PA} P_A} \ln^2 \left(\frac{Z_{REF}}{Z_O} \right) \right]^{1/3} \quad (3.26)$$

If the inequality in Equation 3.25 is satisfied, then (Z_{REF}/L) is set equal to the right side of Equation 3.25. Substituting this value into the expression for U^* yields:

$$U^* = \frac{2}{3} \frac{k U_{REF}}{\ln \left(\frac{Z_{REF}}{Z_O} \right)} \quad (3.27)$$

and:

$$L = \frac{2(4.7)Z_{REF}}{\ln \left(\frac{Z_{REF}}{Z_O} \right)} \quad (3.28)$$

This approach involves setting minimum limits for the values U^* and L . For example, if $Z_{REF} = 10$ m and $Z_O = 0.1$ m, then the corresponding value for L is 20.4 m. For a wind speed, $U_{REF} = 1$ m/s, this value of L corresponds to a minimum value for U^* of 0.058 m/s. The existence of these minimum values imply that a minimum level of turbulence always exists in the stable boundary layer.

3.1.6 Wind Speed Variation With Height

Due to surface friction, the wind speed normally tends to increase with increasing height above the ground. In the absence of an observed wind speed profile, a power law wind relationship is frequently used to estimate wind speeds at heights greater than Z_{REF} (Irwin, 1979):

$$U = U_{REF} \left(\frac{Z}{Z_{REF}} \right)^p \quad (3.29)$$

where

U = wind speed at height Z (m/s)
 U_{REF} = wind speed at height Z_{REF} (m/s)
 p = power law exponent dependent on surface roughness (Z_o) and atmospheric stability.

The method for calculating the exponent p is presented in Table 3.5 (Irwin, 1979). The estimation of the Monin-Obukhov length from Equations 3.32 and 3.35 is independent of previous estimates of the Monin-Obukhov length (Equations 3.16 and 3.20) to facilitate the use of the power law wind profile in the estimation of plume rise (Section 4.3). For this reason, the Monin-Obukhov length in Table 3.5 is designated by the symbol " L_I " instead of " L ". The method given in Table 3.5 allows the exponent p to be a continuous function of the surface roughness Z_o .

Following the recommendation of Hanna (1981), the wind speed calculated by this model is never allowed to exceed the wind speed at 100 m elevation since exponents are empirically determined from tower observations whose vertical heights seldom exceed 100 m. Irwin (1979) also indicated that the power law wind profile will not perform well for heights in excess of 100 m during extremely stable or unstable conditions. A minimum elevation of 1 m is used in the power law. The wind speed for elevations less than 1 m is assumed to be the value calculated at a height of 1 m.

Table 3.5

Estimation of the Wind Speed Power Law Exponent (p).

Unstable Conditions	
$p = \left[\left(1 - 15 \frac{Z_{AVG}}{L_t} \right)^{1/4} \left\{ \ln \left(\frac{Z_{AVG}}{Z_o} \right) + \ln \left[\frac{(\zeta_o^2 + 1)(\zeta_o + 1)^2}{(\zeta^2 + 1)(\zeta + 1)^2} \right] + 2(\tan^{-1} \zeta - \tan^{-1} \zeta_o) \right\} \right]^{-1}$	(3.30)
where:	
$\zeta = \left(1 - 15 \frac{Z_{AVG}}{L_t} \right)^{1/4}$	(3.31)
$\zeta_o = \left(1 - 15 \frac{Z_o}{L_t} \right)^{1/4}$	
The Monin-Obukhov length is estimated from Irwin (1979):	
$\frac{1}{L_t} = -0.002 + 0.018 \log Z_o$	(3.32)
Neutral Conditions	
$p = \log Z_o(0.096 + 0.016 \log Z_o) + 0.24$	(3.33)
Stable Conditions	
$p = \frac{1 + 2Z_{AVG}/L_t}{\ln(Z_{AVG}/Z_o) + 2Z_{AVG}/L_t}$	(3.34)
The Monin-Obukhov length is estimated from Irwin (1979):	
$\frac{1}{L_t} = 0.004 - 0.018 \log Z_o$	(3.35)
Where:	
$Z_{AVG} = \frac{1}{2} \left(\frac{Z_1 + Z_2}{2} + \sqrt{Z_1 + Z_2} \right) = 32.744$	(3.36)
Z_l = lower elevation value = 10 m Z_2 = upper elevation value = 100 m	

3.2 Preprocessor Evaluation

Five years of hourly meteorological data from Calgary International Airport for the period January 1 1980 to December 31 1984 were analyzed to evaluate preprocessor performance. Specifically, hourly values of the following boundary layer parameters were estimated:

- Surface heat flux (H_o)
- Atmospheric stability (Unstable, Neutral or Stable)
- Mixing height (Z_i)
- Friction velocity (U^*)
- Convective velocity scale (W^*).

Where possible, values of the above parameters calculated from the Calgary data were compared to values given in the literature. Calgary International Airport is located amid flat terrain whose surface roughness (Z_o) from visual observation was assumed to be 0.1 m. The non-standard anemometer height of 18.3 m (which differs from the standard height of 10 m) was accounted for.

3.2.1 Surface Heat Flux

Figure 3.2 shows the mean surface heat flux values as a function of time of day and season. Mean values during night-time hours are typically -15 W/m^2 and are relatively constant from season to season. During the day, the heat flux values are closely correlated to solar elevation with mean peak values of 13, 117, 178 and 76 W/m^2 occurring in the winter, spring, summer and fall months respectively. The overall maximum and minimum predicted values for surface heat flux are 268 and -27 W/m^2 respectively. Both the maximum and minimum are associated with clear sky conditions. The maximum heat flux occurs around 1300 hours. The time of the peak heat flux corresponds to what has been measured (Van Ulden and Holtslag, 1985).

The predicted mean peak summer value of 178 W/m^2 is consistent with that predicted by Ning and Yap (1986) for Ontario (which ranged from 150 to 180 W/m^2). Similarly, the overall predicted maximum value of 268 W/m^2 is consistent with the 287 W/m^2 value measured by Davison at Suffield (230 km eastsoutheast of Calgary) for clear sky conditions in mid-July (Davison *et al.* 1981).

Ning and Yap (1986) used techniques similar to those used by the preprocessor to estimate their boundary layer parameters. Their results are presented here as a verification that the independent application of the same approach can produce values which are similar to each other (after accounting for geographical differences between Alberta and Ontario).

3.2.2 Atmospheric Stability

On the average, unstable, neutral and stable conditions were predicted to occur 22, 36 and 42 percent of the time, respectively. Figure 3.3 shows the predicted distribution of atmospheric stability conditions as a function of time of day.

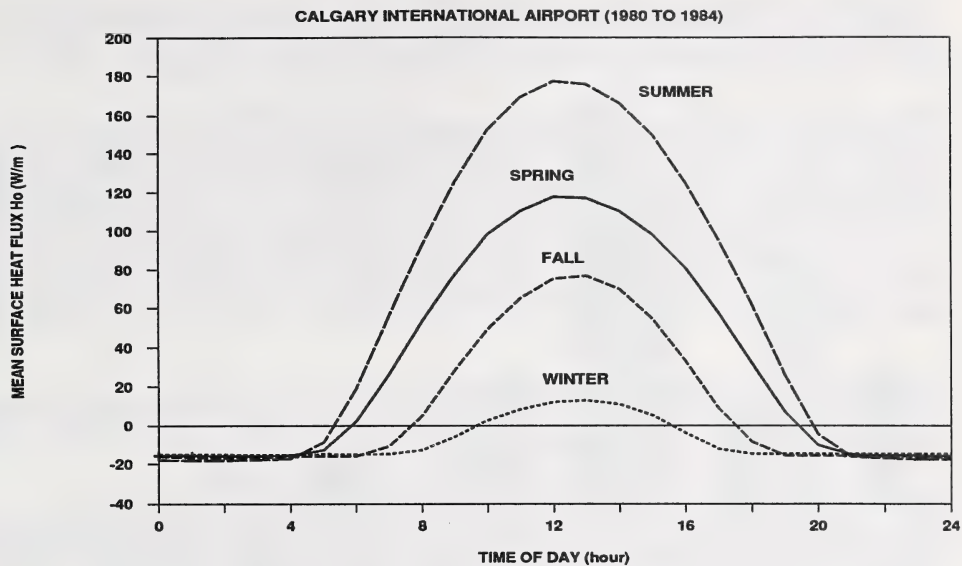


FIGURE 3.2

Predicted Mean Surface Heat Flux (H_o) as a Function of Season and Time of Day.

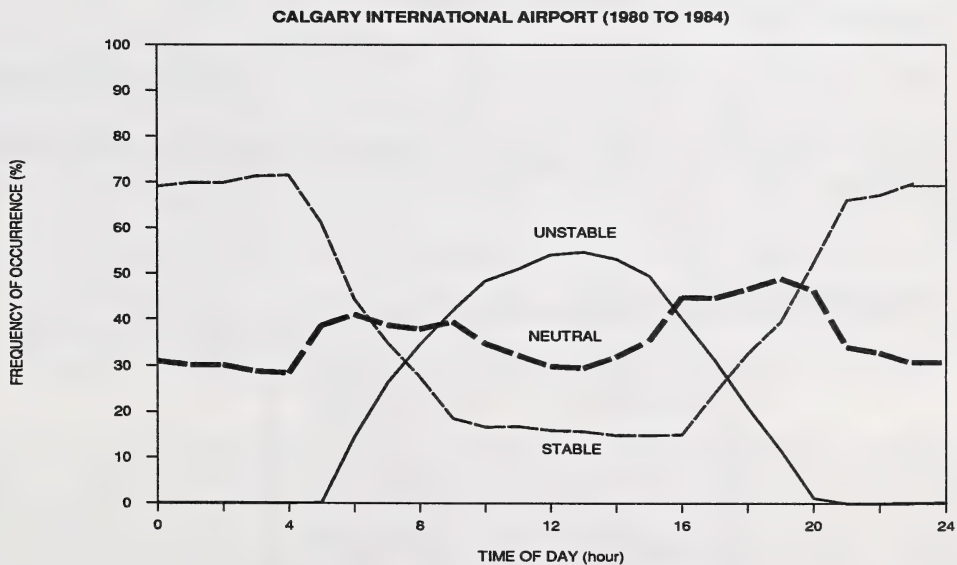


FIGURE 3.3

Predicted Atmospheric Stability Class Frequency as a Function of Time of Day.

As expected, unstable conditions occur during day-light hours and stable conditions are primarily associated with night-time conditions. Neutral conditions can be expected any time of the day with a bias to the night-day and day-night transition hours.

The preprocessor stability classes estimates can be compared to the more familiar Pasquill stability classes. Pasquill (1961) devised an atmospheric typing scheme which considers unstable conditions (Classes A, B and C), neutral conditions (Class D) and stable conditions (Classes E and F). The occurrence of these classes can be estimated from a method proposed by Turner (1970) which is based on routine airport observations and considers wind speed and a net radiation index. This approach has been formalized in a computer program called STAR which is used to estimate a joint frequency distribution of stability class, wind speed and wind direction.

The preprocessor estimates of the Monin-Obukhov length (L) can be related to the Pasquill classes from a nomogram given by Golder (1972). For a surface roughness of 0.1 m, the relationships in Table 3.6 were used.

Figure 3.4 compares the Pasquill stability class frequency distributions predicted using the above relationships with the more familiar STAR approach. Both methods were based on Calgary meteorological data for the same period (1980 to 1984). The STAR approach predicts unstable, neutral and stable conditions 18, 52 and 30 percent of the time respectively. The preprocessor method predicts more frequent occurrences of unstable conditions. This is supported by Weil (1985) and Weil and Brower (1984) who found that the STAR approach was biased towards neutral conditions when, in fact, the atmosphere was unstable.

The preprocessor fails to predict the occurrence of Stability Class F. For Calgary International Airport (where $Z_{REF} = 18.3$ m and $Z_o = 0.1$ m), the corresponding minimum value for L is 32 m which explains the lack of Stability Class F conditions. The minimum value is a result of the method for handling low wind speeds under stable conditions (Table 3.4). As will be seen later in the report, the Pasquill-Smith plume spreads associated with Pasquill Stability Class F are similar to those predicted by the dispersion modelling system. On this basis the lack of Stability Class F occurrences by the preprocessor can not be seen as a failing.

Table 3.6

Relationship Between Pasquill Stability Class and Monin-Obukhov Length L .

Pasquill Class	Range of L (m)
A	0 to -10
B	-10 to -30
C	-30 to -200
D	>150 and < -200
E	30 to 150
F	0 to 30

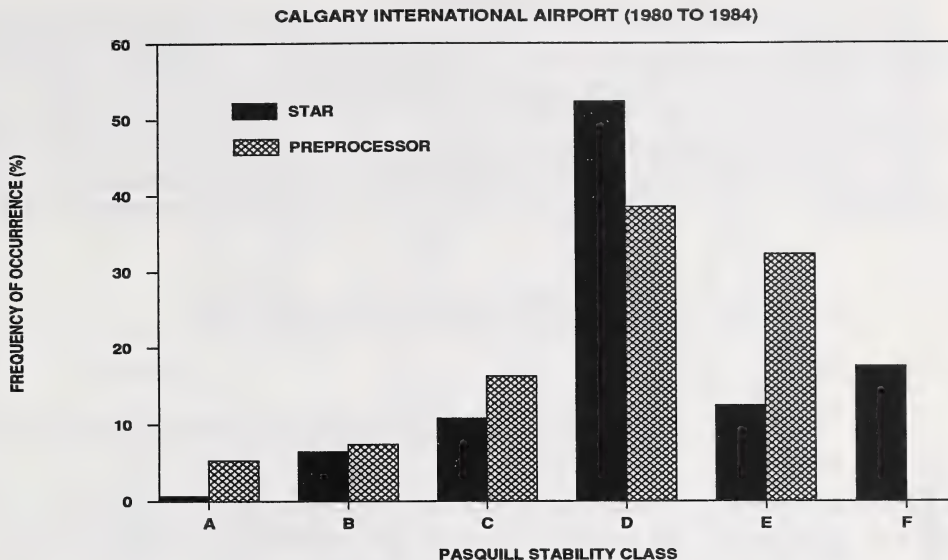


FIGURE 3.4

Comparison of Pasquill Stability Class Predictions.

3.2.3 Mixing Height

Figure 3.5 shows the median predicted mixing height values as a function of time of day and season. The convective mixing layer height estimation was based on the surface temperature alternative (Equation 3.10). During the night, the median mixing layer depths are typically 200 to 400 m. The mixing depth reaches a maximum between 1600 and 1800 hours (depending on season). The shape of the median curves departs from what has been reported elsewhere (Van Ulden and Holtslag, 1985). The figure indicates a gradual rise from the morning minimum value to the late afternoon maximum value. The expected curve, based on the observations reported in Van Ulden and Holtslag (1985), would have reached a maximum value a few hours sooner and levelled off at a constant value before sunset.

The median maximum values predicted by the preprocessor were compared to mixing height value reported by others. Table 3.7 compares the values interpolated for the Calgary area from seasonal maps prepared from four years (1965 to 1969) of upper air observations (Portelli, 1977). During the spring, summer and fall seasons, the preprocessor results are much less than those given by Portelli. Ning and Yap's (1986) mean maximum summer values for Ontario range from 1250 m in the north to 1500 m in the south. Leahey and Hansen (1980) estimated median maximum mixing height values from minisonde data in the Athabasca oil sands region. Their spring, summer, fall and winter values were 1000, 1000, 800 and 270 m, respectively. These spring and summer values are less than those interpolated from the Portelli maps (1200 and 1700 m, respectively).

Portelli based his method on the intersection of the dry adiabat which passes through the surface temperature with the early morning temperature profile. Pendergast (1984) indicates that this method may over predict mixing heights by 50 percent. Leahey and Hansen and the preprocessor indirectly incorporate the dry adiabat intersection assumption. The different mixing height results indicate the uncertainties in the estimation of mixing heights. The accuracy in predicting the lower end of the mixing height range is more critical than that for the higher end range for air quality assessment applications. This is because plume heights (for unignited releases) are expected to be within the first few hundred metres of the surface.

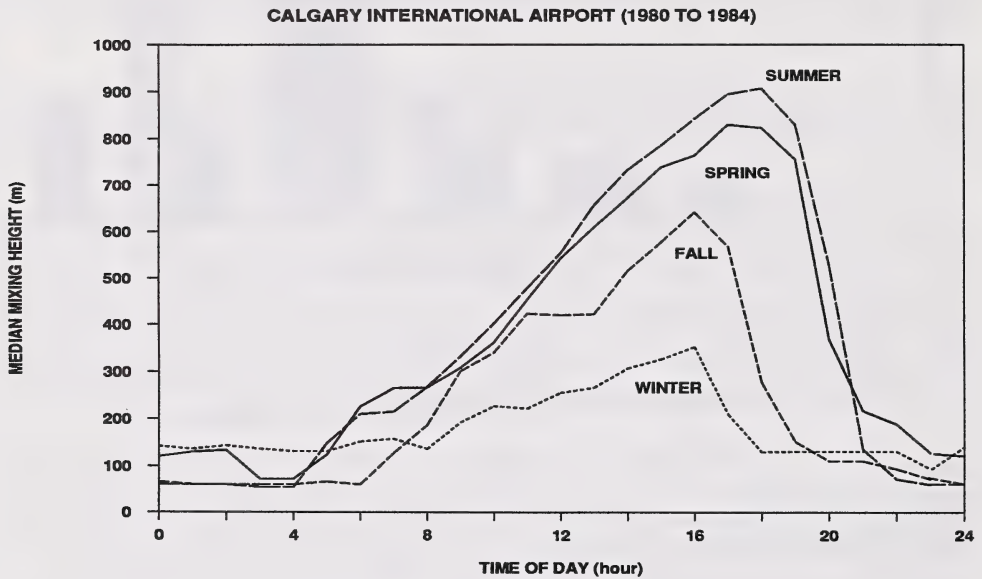


FIGURE 3.5

**Predicted Median Mixing Height (Z_i)
as a Function of Season and Time of Day.**

Table 3.7**Comparison Between Preprocessor and Portelli Estimated Median Mixing Heights
(Calgary International Airport).**

Season	Preprocessor	Portelli
Spring	830 m	1800 m
Summer	906	2100
Fall	642	1100
Winter	351	350

3.2.4 Friction Velocity (Mechanical Turbulence)

For neutral conditions the ratio of U_{REF}/U^* has a mean value of 13 for the selected Calgary International Airport conditions. For unstable conditions, the ratio decreases to a mean value of 10 and for stable conditions, the ratio increases to a mean value of 17.

Figures 3.6 and 3.7 show the frequency of occurrence of wind speed (U_{REF}) and friction velocity (U^*). The wind speed values given in Figure 3.6 include those hours during which calm conditions were reported whereas Figure 3.7 excludes those hours. Figures 3.6 and 3.7 are therefore based on 43 823 and 40 184 hours of data, respectively. Friction velocity values are typically less than 0.5 m/s. For neutral conditions, a friction velocity of 0.5 m/s corresponds to a wind speed of 6.5 m/s. This is consistent with the wind speed frequency distribution where most of the winds are less than 6.5 m/s.

3.2.5 Convective Velocity Scale (Convective Turbulence)

Figure 3.8 shows the convective velocity scale frequency distribution for unstable conditions. Convective velocity values occur most frequently in the 1.1 to 1.7 m/s range. A convective velocity of 1.7 m/s is consistent with a surface heat flux of 170 W/m² and a mixing height of 1000 m. The convective velocity values shown in the figure are consistent with those presented by Ning and Yap (1986) where the mean maximum values for Ontario were found to range from 1.7 to 1.9 m/s. Larger values of W^* result in the plume breaking up faster near the source due to increased turbulence.

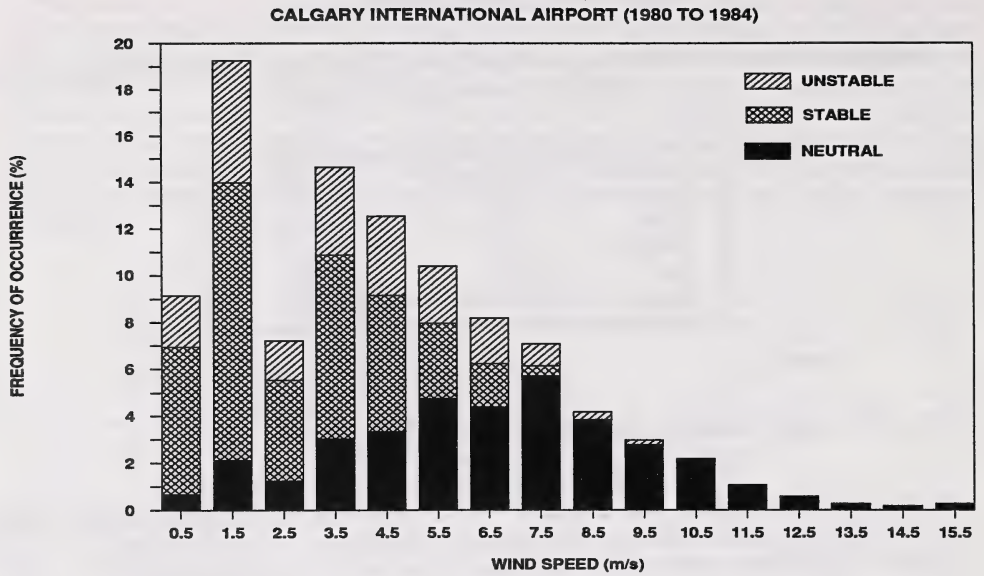


FIGURE 3.6
Observed Wind Speed (U_{REF}) Frequency.

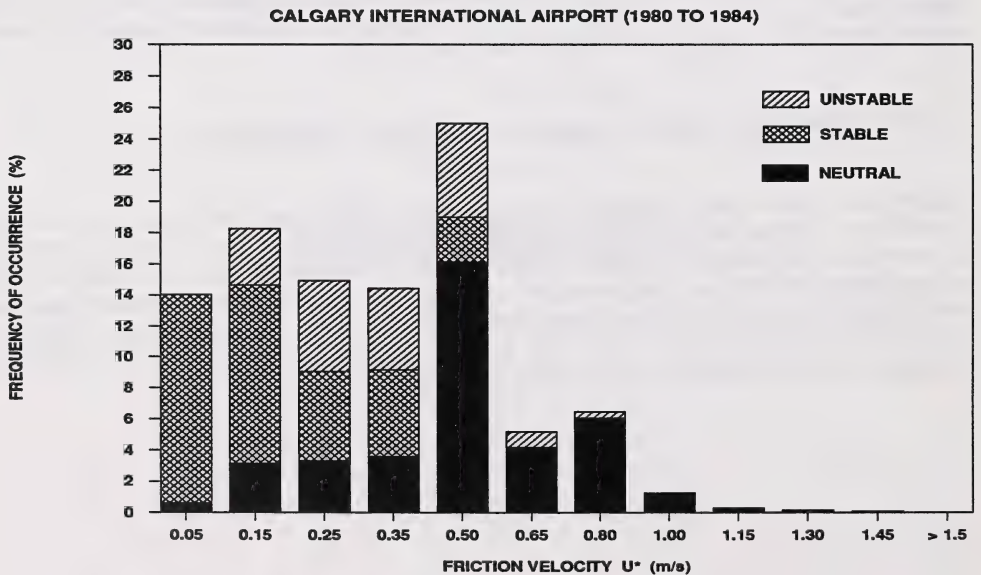


FIGURE 3.7
Estimated Friction Velocity (U^*) Frequency.

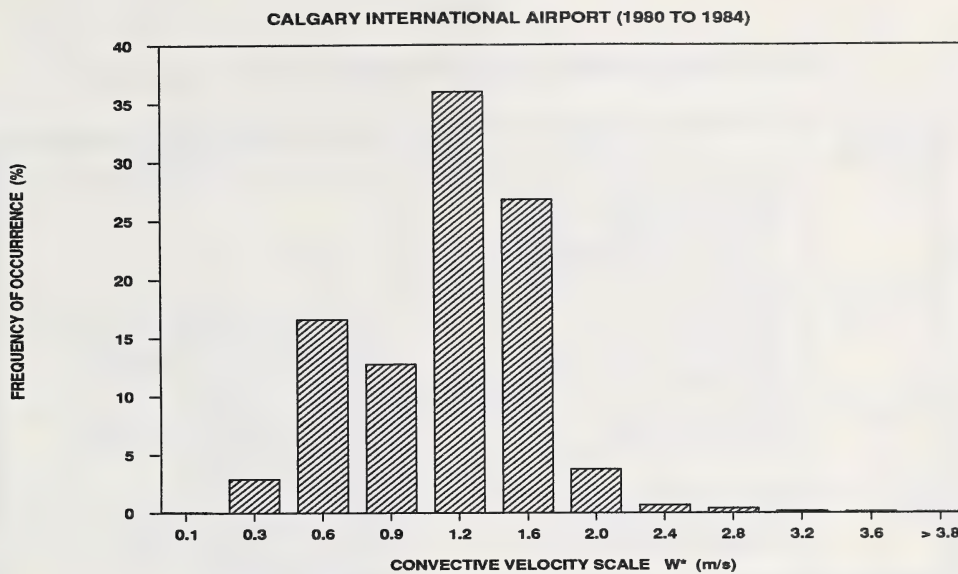


FIGURE 3.8

Estimated Convective Velocity Scale (W^*) Frequency.

3.3 Summary

The meteorological preprocessor can be used to determine the magnitude and frequency of occurrence of planetary boundary layer (PBL) parameters from routine airport observations. The meteorological preprocessor can also be used to determine realistic PBL parameter combinations for evaluation. The independent parameters required by GASCON2, and the dependent parameters calculated by GASCON2 are summarized in Table 3.8. The dependent parameters are estimated from the relationships given in Section 3.1. The design of the preprocessor incorporates our current understanding of boundary layer processes.

The preprocessor was applied to five years of data from Calgary International Airport. The predicted diurnal variations of the heat flux (H_o), stability class and mixing height (Z_i) are qualitatively consistent with what is intuitively expected in the boundary layer. The shape and the magnitude of the predicted mixing height values, however, differ from those reported elsewhere. Predicted values of friction velocity (U^*) and convective velocity scale (W^*) are similar to values reported elsewhere in the open literature.

More detailed and careful meteorological observations are required to confirm the preprocessor predictions for Alberta using AES weather observations. The physics embodied in the preprocessor makes a number of simplifying assumptions. Until better observations are available, however, these simplifying assumptions are not seen as the limiting factor in obtaining better PBL parameters.

Table 3.8**Meteorological Boundary Layer Parameters Used by GASCON2.**

Stability	Input	Calculation
All	Surface Roughness (Z_o) Reference Height (Z_{REF}) Ambient Temperature (T_{AO}) Ambient Pressure (P_{AO})	
Unstable	Wind Speed (U_{REF}) Surface Heat Flux (H_o) Convective Mixing Height (Z_i)	Convective Velocity Scale (W^*) Monin-Obukhov Length (L) Friction Velocity (U^*)
Neutral	Wind Speed (U_{REF}) Surface Heat Flux (H_o)	Monin-Obukhov Length (L) Friction Velocity (U^*) Mixing Height (Z_i)
Stable	Wind Speed (U_{REF}) Surface Heat Flux (H_o)	Monin-Obukhov Length (L) Friction Velocity (U^*) Mixing Height (Z_i)



4 MODEL FRAMEWORK

The GASCON2 model has been subdivided into a series of inter-dependent modules which can be used to estimate ground level concentrations, potential hazard zones, probability of lethality and potential fatalities corresponding to a given release scenario. As shown in Figure 4.1, these modules include the:

- Mass Emission Rate,
- Jet Expansion,
- Plume Rise,
- Transient Release,
- Passive Dispersion, and
- Consequence Modules.

The Mass Emission Rate Module (Section 4.1) estimates the sour gas release rate from well blowouts and pipeline ruptures. The well blowout portion of the module is trivial since the release rate is assumed to be constant with time. In contrast, the release rate from a pipeline rupture is a highly transient process, typically lasting no more than a few minutes.

The Jet Expansion Module (Section 4.2) simulates the initial behavior of the gas after its release to the atmosphere. Five "regions" are addressed:

- the Stagnation Zone which considers conditions at the jet exit,
- the Pressure Equalization Zone which considers the expansion of gas from the sonic, underexpanded state to atmospheric pressure,
- the Drag Zone which considers obstructions that reduce the gas velocity,
- the Entrainment Zone which considers entrainment of ambient air into the jet, and
- the Combustion Zone which considers the potential ignition of the escaping gases.

These five regions of gas behavior are modelled as series processes.

The Plume Rise Module (Section 4.3) estimates the momentum and buoyancy rise of the jet after the jet expansion stage. Unlike usual plume rise estimates, this module can address non-vertical releases explicitly.

The Transient Release Module (Section 4.4) calculates an effective mass release rate for pipeline releases. The use of an effective mass release rate in the Passive Dispersion Module allows steady state dispersion formulations to be adopted for transient pipeline releases.

The Passive Dispersion Module (Section 4.5) estimates ground level plume concentrations as a function of distance from the release point. Unstable, neutral and stable atmospheres are considered. The turbulence in the atmosphere is allowed to vary continuously. Dispersion from elevated and surface releases are considered differently.

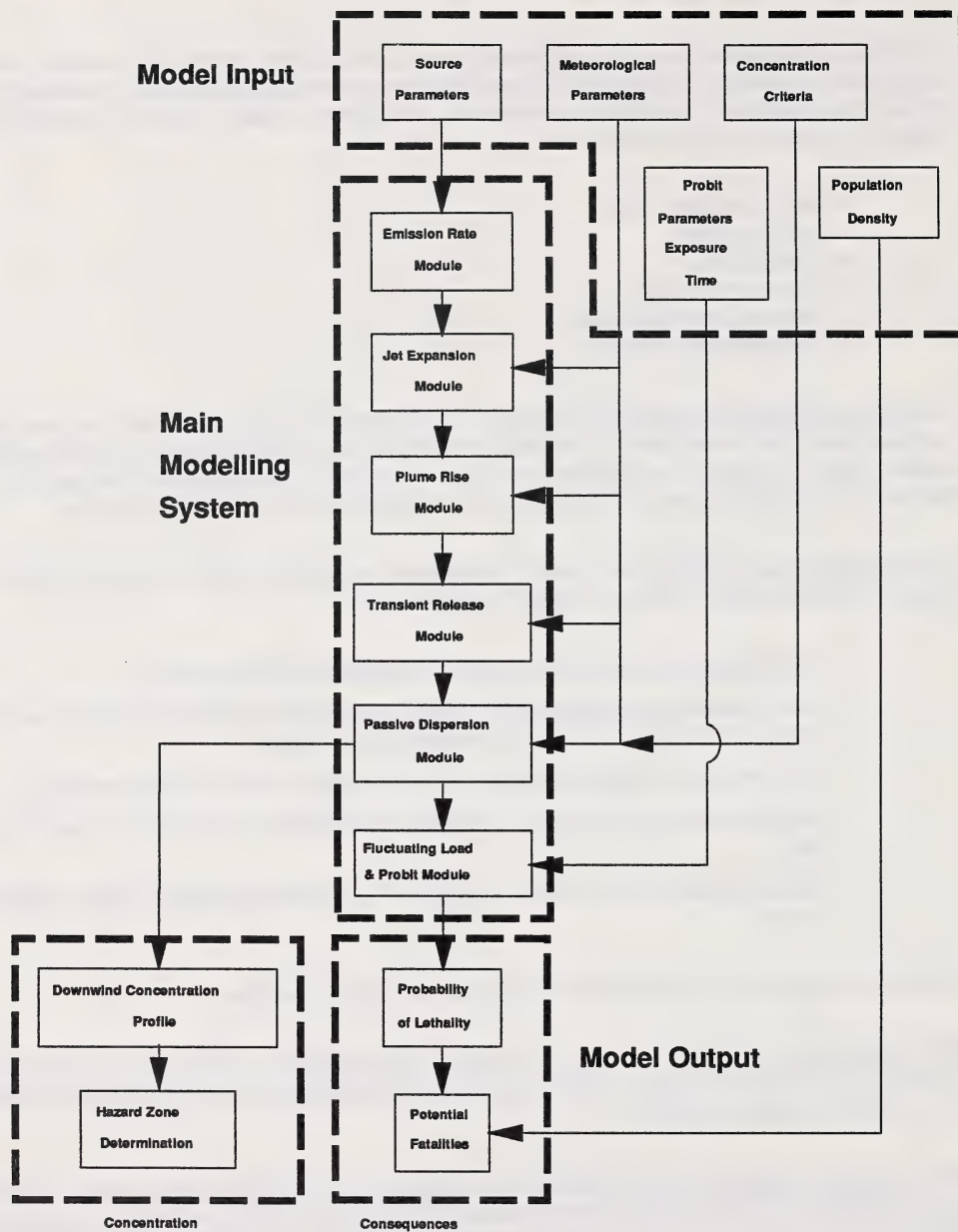


FIGURE 4.1
Detailed GASCON2 Modelling Framework.

Four model outputs are generated. The first two deal with concentrations and result from the Passive Dispersion Module. This output responds to the question: *For a given uncontrolled sour gas release, what is the concentration of toxic gas (H₂S or SO₂) at locations downwind of a release point, and what is the potential hazard zone where concentrations exceed a critical level?*

The Fluctuating Load and Probit Module (Section 4.6) estimates the consequences downwind of a given uncontrolled sour gas release. Fluctuating load analysis accounts for fluctuations in concentration from the average value estimated in the Passive Dispersion Module. Probit analysis estimates the likelihood of fatalities in a population due to the exposure of H₂S.

The last two outputs deal with consequences and result from the Fluctuating Load and Probit Module. This output responds to the question: *For a given uncontrolled sour gas release, what is the probability of receiving a lethal toxic load (dose) of H₂S at locations downwind of the release point and what would the potential fatalities be?*

By knowing the frequency of uncontrolled sour gas releases and the probability that the release will result in lethal conditions to the human population in the vicinity of the release, the threat (or risk) posed by that uncontrolled release can be estimated. Volume 6 (Alp *et al.* 1990) provides details on the methods used to calculate risk. However, the most beneficial use of GASCON2 is to assess the effectiveness of various design and operation changes implemented to reduce risk. In assessing the relative risk changes for two alternate designs, many of the uncertainties cancel, because they appear in both alternatives. This makes GASCON2 inherently better at assessing alternatives than in providing absolute risk values.

4.1 Mass Emission Rate Module

The release rate of sour gas from potential uncontrolled discharges may be continuous (steady state) in the case of well releases or may be transient in the case of pipeline releases. Should an ESD valve fail at the well, then the release from a pipeline may have an initial transient component followed by a decay to a non-zero steady-state value.

Physical properties of the sour gas stream are required by the mass emission rate module (and by the jet expansion module). Specific properties of a gas stream "I" of known composition include the molecular mass (M_{WI}), heat of combustion (Q_{HI}), specific heat at constant pressure (C_{PI}) and the particular gas constant (R_I). Table 4.1 indicates how these properties are calculated from the gas composition.

4.1.1 Continuous Well Release

The deliverability of a well is usually expressed as a daily volume flow at a standard temperature and pressure of 15 °C and 101.3 kPa respectively. Of primary interest to the current dispersion modelling exercise, however, is the mass release rate of sour gas, denoted by $\dot{m}_E$:

$$\dot{m}_E = \frac{\rho_{EO} \dot{V}}{86,400} \quad (4.1)$$

where: $\dot{V}$ = volume flow rate of sour gas (m³/d)
 ρ_{EO} = density of sour gas at standard conditions (kg/m³)
 $\dot{m}_E$ = mass flow rate of gas (kg/s).

Since the volume flow rates are usually quoted for standard conditions (15 °C and 101.3 kPa), the density may be estimated from the ideal gas law:

$$\rho_{EO} = \frac{(101.3)(10^3) M_{WE}}{(288) 8314} \quad (4.2)$$

where M_{WE} = molecular mass of the discharging gas (kg/kmole).

The user must input the mass flow rate of gas (kg/s) for steady releases. The event or exposure time for continuous well releases is meteorology dependent. A minimum of 60 minutes and a maximum of 180 minutes is recommended.

Table 4.1
Example of Gas Property Calculations.

For a gas stream of known composition "I", the molecular mass M_{WI} of the combined gas stream can be calculated as the sum of the individual molecular masses weighted according to the individual mole fraction. As an example, for a typical sour gas stream:

Component	Mole Fraction	Molecular Mass	Product
C ₁	0.550	16.043	8.82
C ₂	0.005	30.070	0.15
C ₃	0.001	44.097	0.04
C ₄	0.001	58.123	0.06
H ₂ S	0.300	34.076	10.22
CO ₂	0.123	44.010	5.41
N ₂	0.020	28.013	0.56
Total:			25.27

The molecular mass of the gas stream is 25.27 kg/kmole. The heat of combustion (Q_{HI}) and the specific heat at constant pressure (C_{PI}) are calculated in a similar manner. Values for the individual molecular mass, heats of combustion and specific heats at constant pressure can be obtained from the SI Engineering Data Book (Gas Processors Suppliers Association, 1980).

The particular gas constant R_I (J/(kg K)) of the gas stream is given by:

$$R_I = \frac{R_U}{M_{WI}} \quad (4.3)$$

where R_U = universal gas constant (8314.4 J/(kmole K)).

The ratio of specific heats for the gas stream is from the definition:

$$k_I = \frac{C_{PI}}{C_{VI}} = \frac{C_{PI}}{C_{PI} - R_I} \quad (4.4)$$

The user inputs M_{WE} , C_{PE} and Q_{HE} and the program calculates R_I and k_I as required.

4.1.2 Transient Pipeline Release

In contrast to well blowouts, the release of sour gas from a ruptured pipeline is a highly transient process, typically lasting no more than a few minutes. The nature of the release is dependent on the operating pressure of the pipeline, the size of the rupture and the length of pipeline isolated by emergency shutdown (ESD) valves. Since the volume of gas in the isolated section of ruptured pipeline is limited, the release is characterized by decreasing line pressure and decreasing mass flow rate.

Bell (1978) introduced a "double exponential" model for the blowdown of a pressurized pipeline:

$$\dot{m}_E = \frac{\Gamma \dot{m}_O}{(1 + \eta)} \left[\exp\left(-\frac{t}{\eta^2 \epsilon}\right) + \eta \exp\left(-\frac{t}{\epsilon}\right) \right] \quad (4.5)$$

where:

$\dot{m}_E$ = mass release rate (kg/s)

$\dot{m}_O$ = initial gas release rate (kg/s) at time $t = 0$ s

Γ = inertial delay factor (≤ 1.0)

t = time after the release (s)

$\eta = M_T / (\epsilon \Gamma \dot{m}_O)$ = mass conservation factor

M_T = total mass to be released (kg)

ϵ = time constant (s).

The initial release rate $\dot{m}_O$ may be calculated from the adiabatic choked flow condition:

$$\dot{m}_O = \frac{P_O A_E \sqrt{k_E}}{\sqrt{R_E \bar{Z}_E T_O}} \left[\frac{2}{k_E + 1} \right]^{\frac{1}{2} \{ (k_E + 1) / (k_E - 1) \}} \quad (4.6)$$

which may be found in any standard reference text on compressible flow (e.g., Shapiro, 1953). In this equation:

P_O = gas pressure in pipeline before rupture (Pa)

A_E = cross sectional area of rupture (m^2)

k_E = ratio of specific heats for the pipeline gas (C_p/C_v)

R_E = gas constant for the pipeline gas ($\text{J}/(\text{kg K})$)

T_O = temperature of gas in pipeline before rupture (K)

$\bar{Z}_E$ = gas compressibility at the exit (assumed to be 1.0).

The time constant ε has been shown by Wilson (1989) to be given by:

$$\varepsilon = \frac{2}{3} \frac{l}{C_o} \left(\frac{d}{k_E F l} \right) \left(\frac{A_p}{A_E} \right)^3 \left(\frac{k_E + 1}{2} \right)^{\left[\frac{3}{2} \left(\frac{k_E + 1}{k_E - 1} \right) \right]} \left[\left(1 + \left(\frac{k_E + 1}{2} \right)^{\left(\frac{k_E + 1}{k_E - 1} \right)} \left(\frac{A_E}{A_p} \right)^2 \frac{k_E F l}{d} \right)^{\frac{3}{2}} - 1 \right] \quad (4.7)$$

where:

- l = length of pipeline between valves ESD (m)
- C_o = speed of sound in pipeline gas before rupture (m/s)
- F = pipeline friction factor
- d = pipeline inside diameter (m)
- A_p = cross sectional area of pipe (m²).

The user inputs the pipeline inside diameter and the hole size as a fraction of pipeline flow area (A_E/A_p).

The mass conservation factor η insures that the total mass to be released is recovered upon the following integration:

$$\int_0^{\infty} \dot{m}_E(t) dt = M_T \quad (4.8)$$

The total mass released is determined by:

$$M_T = \frac{l_{EFF} A_p P_o}{R_E \bar{Z}_C T_o} \quad (4.9)$$

where:

- $\bar{Z}_C$ = pipeline gas compressibility prior to the rupture
- l_{EFF} = effective pipeline length to allow for the extra gas released during the time taken for the ESD valves to fully close.
= $l \cdot (1 + \delta)$.

The δ value represents the additional mass and is expressed as a fraction of the total mass of the gas contained in the isolated segment of the pipeline. Numerical modelling studies have shown that this excess can be of the order of 0.3 for a valve closure time of 30 s, a pipeline length of 1600 m, and a pipeline diameter of 15.5 cm (APIGEC, 1978). That is, the gas released to the atmosphere for this example is 1.3 times that contained within the 1600 m segment of the pipeline.

Sonic velocity in the pipeline gas is given by:

$$C_o = \sqrt{k_E R_E \bar{Z}_C T_o} \quad (4.10)$$

The event time t_E for transient releases is the time required to release 99% of the total mass (M_T), and is determined by solving the following for t_E in seconds and converting to minutes:

$$\int_0^{t_E} \dot{m}_E(t) dt = 0.99M_T \quad (4.11)$$

The expression for the initial mass rate (Equation 4.6) is based on adiabatic choked flow theory. At the onset of a pipeline rupture, an expansion wave travels down the pipeline at the local speed of sound. At the rupture exit, the gas flow behind the wave accelerates to sonic velocity. Typically, the region of significant gas acceleration is confined to a length of pipeline approximately 200 diameters upstream of the rupture point. This region of the flow is assumed to be determined by an adiabatic process in which the sum of the internal and kinetic energies of the flow remains constant.

Beyond approximately 200 diameters upstream of the rupture point, the gas flow is characterized by a relatively small change in gas velocity. This, coupled with the fact that most sour gas pipelines are buried in the ground which acts as a thermal reservoir, indicates that much of the pipeline gas during the entire blowdown time is undergoing an isothermal process. For most of the blowdown time and for almost all the pipeline length, the pipeline is releasing gas as a fixed volume, isothermal (decreasing pressure) containment vessel. The expression for the time constant (Equation 4.7) is based on isothermal flow theory.

The preceding two paragraphs justify adopting adiabatic assumptions near the exit section of the pipeline ($\bar{Z}_E = 1.0$) and isothermal assumptions upstream of the exit section of the pipeline.

The double exponential mass release model has been tested against the experiments of Dielwart *et al.* (1979) by Wilson (1981) and subsequently used by Choukalos (1982) in the Alberta Environment risk model. Its use is based on two important considerations:

- An exponential decay in mass flow is the exact solution to an isothermal fixed length blowdown after the rupture expansion wave reaches the pipeline ESD valve.
- The satisfactory agreement of the model with the release rate time history measured in a study conducted by APIGEC (Dielwart *et al.*, 1979). Wilson (1981) found the best agreement using $\Gamma = 0.5$ in the double exponential relation.

In the light of the above considerations, the double exponential model of Bell (1978) and Wilson (1981) has been selected for implementation in this work.

4.1.3 Continuous Pipeline Release

If a pipeline were to rupture and the ESD valve(s) between the ruptured segment and the well were to fail, the release of the sour gas would be characterized by an initial transient peak which would decay to a steady state value. In this event, the mass release rate is approximated by:

$$\dot{m}_E(t) = \text{MAX}[\dot{m}_{E,T}(t), \dot{m}_{E,S}] \quad (4.12)$$

where $\dot{m}_{E,T}(t)$ is the transient mass release rate and $\dot{m}_{E,S}$ is the steady state mass release rate.

The mass release profile represented by the above equation decays exponentially to time t_s and is constant thereafter. The time t_s is given by the solution to the equation:

$$\frac{\Gamma \dot{m}_O}{(1 + \eta)} \left[\exp\left(-\frac{t_s}{\eta^2 \epsilon}\right) + \eta \exp\left(-\frac{t_s}{\epsilon}\right) \right] = \dot{m}_{E,S} \quad (4.13)$$

Caution should be used in specifying the event time t_E for continuous pipeline releases as the consequences associated with high concentrations due to the initial transient can be artificially reduced by selecting large event times corresponding to a steady release.

4.2 Jet Expansion Module

Throughout a well blowout, and for virtually the entire duration of a pipeline blowdown, the discharging gas experiences choked flow conditions at the rupture exit. The expansion of the gas from the sonic, underexpanded state to atmospheric pressure, the influence of drag, the entrainment of ambient air and the potential combustion of gas are treated in the jet expansion module as a series of simplified processes. The parameterization of these processes required extensive review of existing methods and the development of practical working equations from basic principles. This effort constituted original model development specifically undertaken for the present model.

Figure 4.2 shows the exit of a gas jet at sonic velocity from an opening ("E"). The jet undergoes an adiabatic expansion due to the equalization of the exit pressure to atmospheric pressure ("Q"). Drag and air entrainment cause a deceleration of the jet to sub-sonic velocity ("D" and "S"). The possible ignition of the jet causes the creation of combustion products and the generation of heat which raises the jet temperature ("C").

A major assumption in the above view of the jet expansion process is that the five "regions" may be modelled as series processes, rather than simultaneous processes. In addition to this, a further assumption is made that the jet may be treated in a one-dimensional, quasi-steady fashion.

4.2.1 Stagnation Zone

At the exit, or rupture, there are certain known quantities which may be regarded as inputs:

- M_{WE} = molecular mass of the discharging gas at "E" (kg/kmole)
- C_{PE} = specific heat at constant pressure of the gas at "E" (J/(kg K))
- T_O = stagnation temperature of the gas before discharge (K)
- A_E = area of the exit or rupture (m^2)
- $\dot{m}_E$ = the mass flow rate of gas discharge (kg/s)
- R_E = gas constant of the discharging gas (J/(kg K))
- k_E = ratio of specific heats of discharging gas.

From Shapiro (1953) the pressure (P_E) at the exit of an adiabatic choked flow discharge is given by:

$$P_E = \frac{\dot{m}_E}{A_E} \left[\frac{R_E T_O}{k_E} \left(\frac{2}{k_E + 1} \right) \right]^{1/2} \quad (4.14)$$

Note that for large steady flows, the resulting exit pressure may be higher than the well can sustain. The choked flow condition constrains the exit velocity to be sonic:

$$V_E = \left[k_E R_E T_O \left(\frac{2}{k_E + 1} \right) \right]^{1/2} \quad (4.15)$$

By conservation of mass, the gas density at the exit may be determined:

$$\rho_E = \frac{\dot{m}_E}{A_E V_E} \quad (4.16)$$

The ideal gas law requires the gas temperature at the exit to be:

$$T_E = \frac{P_E}{\rho_E R_E} = \frac{2T_O}{k_E + 1} \quad (4.17)$$

The conditions at the exit P_E , V_E , ρ_E and T_E can therefore be defined from the preceding relationships.

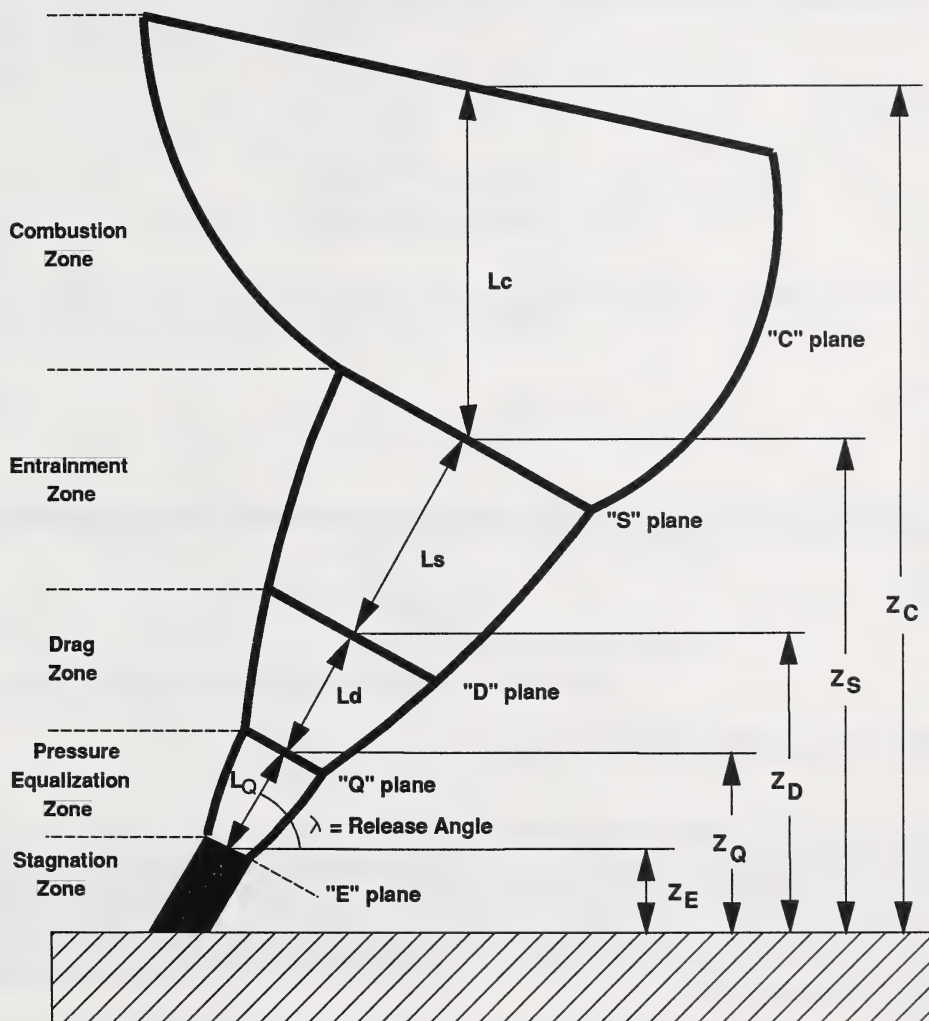


FIGURE 4.2
Jet Expansion Region.

Subsonic Flow Conditions

When the predicted pressure at "E" is less than surface atmospheric pressure, Equation 4.13 is not valid. In this event, which can occur for small leaks or for transient mass discharges at large times, the conditions at the "E" plane are given as:

$$P_E = P_{AO} \quad (4.18)$$

$$T_E = \left\{ -C_{PE} + \left[C_{PE}^2 + \frac{2C_{PE}T_O\dot{m}_E^2R_E^2}{A_E^2P_{AO}^2} \right]^{1/2} \right\} \frac{A_E^2P_{AO}^2}{\dot{m}_E^2R_E^2} \quad (4.19)$$

$$\rho_E = \frac{P_{AO}}{R_ET_E} \quad (4.20)$$

$$V_E = \frac{\dot{m}_E}{\rho_E A_E} \quad (4.21)$$

The equation for P_E assumes no pressure drop across the rupture. It is worthy of note that the expression for T_E is derived from the energy balance:

$$\dot{m}_E C_{PE} T_O = \dot{m}_E C_{PE} T_E + \frac{\dot{m}_E V_E^2}{2} \quad (4.22)$$

4.2.2 Pressure Equalization Zone

Birch *et al.* (1984) studied the behavior of underexpanded compressible sonic jets of natural gas into quiescent air. They predicted the concentration field arising from the expansion of these jets by treating them as classical sub-sonic jets with an appropriate length scale called the "pseudo-diameter". The pseudo-diameter is a theoretical concept describing the effective size of the jet source, which when substituted into the equations defining a sub-sonic round jet, adequately describes the behavior of the jet flow. Their predictions compared favourably with experimental data.

The area of the jet at the "Q" plane (A_Q) shown in Figure 4.2 is given by the circular area defined by the pseudo-diameter. Specifically, the condition of the jet at the "Q" plane arises from the consideration of the area that would be occupied by the same mass flow as at the exit plane (the "E" plane), at the same temperature as that at the exit plane, at ambient pressure and at uniform sonic velocity.

At the exit conditions (the "E" plane), the gas jet is considered to be "underexpanded" since the exit pressure may exceed atmospheric (ambient) pressure by an order of magnitude or so. As the jet pressure equilibrates to atmospheric pressure, the jet expands. At "Q" in Figure 4.2, the jet has undergone no changes in composition, thus:

$$\begin{aligned}
M_{WQ} &= M_{WE} \\
C_{PQ} &= C_{PE} \\
R_Q &= R_E \\
k_Q &= k_E
\end{aligned}
\tag{4.23}$$

At "Q" the ideal gas law is applied:

$$\rho_Q = \frac{P_{A0}}{R_Q T_Q} \tag{4.24}$$

where $P_Q = P_{A0}$ (ambient surface pressure) has been applied.

Assuming adiabatic conditions, the application of the conservation of energy between the "Q" plane and the stagnation conditions at "E" gives:

$$T_Q = \frac{2T_0}{k_Q + 1} = T_E \tag{4.25}$$

The jet velocity at "Q" is considered to be sonic:

$$V_Q = C_Q \equiv \sqrt{k_Q R_Q T_Q} = V_E \tag{4.26}$$

Continuity of mass (with no air entrainment) demands that:

$$A_Q = A_E \frac{\rho_E V_E}{\rho_Q V_Q} = A_E \frac{P_E}{P_{A0}} \tag{4.27}$$

These equations form a closed set of equations for the four unknowns (A_Q , V_Q , ρ_Q , and T_Q) and apply to sonic and subsonic conditions. The length of the pressure equalization zone (L_Q) is expected to be of the order of a few pipe diameters and is neglected in estimating the height of the plume above the ground.

Momentum has not been conserved in the above analysis, as the reduction in pressure has not been converted into an increase in velocity. Wilson (1981) has shown that the gas can be accelerated up to a Mach number of about 2 for large pressure ratios. The analysis used is conservative as the momentum flux is constant from the "E" to the "Q" plane. Momentum flux determines the plume rise due to momentum. If the acceleration of the gas to beyond sonic velocity was accounted for, the momentum flux would increase by up to a factor of 1.7 times.

4.2.3 Drag Zone

Once the jet has expanded to atmospheric pressure at the "Q" plane, its speed is further reduced by drag forces and/or entrainment of air. Drag could be caused by an obstruction such as equipment or by impingement with the walls of the crater which results from a pipeline rupture. The methods of Wilson (1981) were used to model the effects of drag.

During drag deceleration, there is no air entrainment into the jet and the drag force acts uniformly over the jet. This is equivalent to assuming that the jet passes through a porous mesh, located at the "D" plane in Figure 4.2, which slows it down and thus increases the flow area. At the "D" plane, one can define the following:

$$\begin{aligned} M_{WD} &= M_{WQ} \\ R_D &= R_Q \\ C_{PD} &= C_{PQ} \\ k_D &= k_Q \\ P_D &= P_{AO} \end{aligned} \quad (4.28)$$

The reduction in momentum, assuming no air entrainment, equals the drag force:

$$\dot{m}_E (V_D - V_Q) = \frac{C_D}{4} \dot{m}_E (V_D + V_Q) \quad (4.29)$$

C_D = drag coefficient,

- 0 for an unobstructed jet,
- 1 for side rupture in pipeline crater,
- 2 for bottom rupture in pipeline crater,
- 3 for equipment obstruction.

This equation assumes an average velocity between the "Q" and "D" plane in the estimation of the drag force and can be manipulated to solve for the velocity at "D" (V_D) directly. C_D must be less than 4, otherwise $V_D = 0$.

The conservation of energy for an adiabatic process between "Q" and "D" can be solved for the temperature at the "D" plane:

$$\dot{m}_E C_{PQ} T_Q + \dot{m}_E \frac{V_Q^2}{2} = \dot{m}_E C_{PD} T_D + \dot{m}_E \frac{V_D^2}{2} \quad (4.30)$$

where $\dot{m}_E = \dot{m}_Q = \dot{m}_D$ has been applied. The ideal gas law yields the density of the released gas at the "D" plane:

$$\rho_D = \frac{P_{AO}}{R_D T_D} \quad (4.31)$$

From the conservation of mass, the area at "D" can be determined:

$$A_D = A_Q \frac{\rho_Q V_Q}{\rho_D V_D} = A_Q \frac{V_Q T_D}{V_D T_Q} \quad (4.32)$$

The above equations completely define the required properties at the "D" plane. If the drag coefficient is zero, then V_D , T_D , ρ_D and A_D do not change from the "Q" to "D" plume. The length of the drag zone (L_D) is neglected in estimating the height of the plume above the ground. As noted by Wilson (1981), drag reduces the momentum without adding mass to the jet, while air entrainment adds mass to the jet but does not lower its momentum.

4.2.4 Entrainment Zone

It is clear that a high velocity cannot persist for long in the jet as ambient air entrainment cause the jet to decelerate. At "D" in Figure 4.2, the discharged gas has not changed in composition from the stagnation composition. As air is entrained into the jet, however, the molecular mass (M_{ws}) and the specific heat at constant pressure (C_{ps}) for the gas-air mixture changes (assuming steady state conditions):

$$M_{ws} = \frac{M_{WA} M_{WQ}}{M_{WQ}(\dot{m}_A/\dot{m}_S) + M_{WA}(1 - \dot{m}_A/\dot{m}_S)} \quad (4.33)$$

$$C_{ps} = \left(\frac{\dot{m}_A}{\dot{m}_S} \right) C_{PA} + \left(1 - \frac{\dot{m}_A}{\dot{m}_S} \right) C_{PQ} \quad (4.34)$$

where: M_{WA} = molecular mass of air (28.964 kg/kmole)
 C_{PA} = specific heat at constant pressure for air (1005 J/(kg K))
 $\dot{m}_A$ = mass flow of air entrained between "D" plane and "S" plane (kg/s)
 $\dot{m}_S$ = mass flow of gas-air mixture through the "S" plane (kg/s).

The ratio of specific heats k_s and the gas constant R_s are given by Equations 4.3 and 4.4.

Conservation of mass from the "D" plane to the "S" plane demands that:

$$\dot{m}_s = \dot{m}_E + \dot{m}_A = \rho_s A_s V_s \quad (4.35)$$

where $\dot{m}_E = \dot{m}_D$ has been applied. The conservation of energy for an adiabatic process between "D" and "S" gives:

$$\dot{m}_E C_{PD} T_D + \dot{m}_E \frac{V_D^2}{2} + \dot{m}_A C_{PA} T_{AO} = \dot{m}_S C_{PS} T_S + \dot{m}_S \frac{V_S^2}{2} \quad (4.36)$$

where T_{AO} = ambient surface temperature (K). Note the kinetic energy of entrained air and potential energy have been neglected.

The conservation of momentum dictates that:

$$\dot{m}_E V_D + \dot{m}_A U_D \cos \lambda = \dot{m}_S V_S \quad (4.37)$$

where: U_D = ambient wind speed at height "D" (m/s)
 λ = angle of release with horizontal.

The ideal gas law applied at "S" results in:

$$\rho_S = \frac{P_{A0}}{R_S T_S} \quad (4.38)$$

The jet velocity at "S", in terms of the Mach number (M_S) is:

$$V_S = M_S \sqrt{k_S R_S T_S} \quad (4.39)$$

The previous equations represent a closed set of equations for all the variables at "S" and $\dot{m}_A$, provided the Mach number M_S is specified. The value of M_S effects the "S" plane parameters used in the calculation of buoyancy flux. A maximum recommended value for M_S of 0.3 insures that flow compressibility effects are small. It is also possible to specify M_S too low ($< \sim .01$), resulting in a velocity at "S" less than the wind speed ($V_S < U_D$). The suggested values for M_S are:

$$\begin{aligned} M_S &\sim 0.3 \text{ for a jet} \\ M_S &\sim .01 \text{ for a cloud} \end{aligned} \quad (4.40)$$

Due to the non-linear and coupled nature of these governing equations, the solution of the equation set is best handled iteratively through the method given in Table 4.2.

Once all the relevant variables at "S" are known, it becomes possible to estimate the length of the jet between the "D" and "S" plane in Figure 4.2 using the Taylor hypothesis for jet entrainment:

$$\dot{m}_A = \alpha \rho_{A0} A_{EFF} V_{EFF} \quad (4.41)$$

where: ρ_{A0} = ambient air density at surface (kg/m^3)

$$= \frac{P_{A0}}{R_A T_{A0}} \quad (4.42)$$

α = entrainment constant = 0.13

Table 4.2
Estimation of "S" Plane Parameters.

The procedure may be summarized as follows:

- (1) Assume a value for the entrained mass rate $\dot{m}_A$.
- (2) Calculate $\dot{m}_S$ since $\dot{m}_E$ is known (Equation 4.35).
- (3) Calculate M_{ws} (Equation 4.33).
- (4) Calculate C_{PS} (Equation 4.34).
- (5) Calculate R_S (Equation 4.3).
- (6) Calculate k_S (Equation 4.4).
- (7) Calculate V_S (Equation 4.36 with Equation 4.39 for T_S).
- (8) Calculate the difference between the left-hand side and the right-hand side of the conservation of momentum equation (Equation 4.37).
- (9) As long as the difference calculated in step (8) is significantly different from zero, revise the value for $\dot{m}_A$ and go back to step (2). If the residual is small enough ($< .001 \text{ kg m/s}^2$), terminate the iteration.

This procedure may be treated as a root-finding problem for the residual calculated in step (8) versus the entrained air mass rate $\dot{m}_A$.

- (10) Calculate T_S (Equation 4.39).
- (11) Calculate ρ_S (Equation 4.38).
- (12) Calculate A_S (Equation 4.35).
- (13) Calculate L_S (Equation 4.41 to 4.44)

with V_{EFF} = effective tangential velocity difference (m/s);

$$V_{EFF} = \frac{\left[\dot{m}_E - \frac{\dot{m}_A}{\left(\frac{A_S}{A_D} \right)^{1/2} - 1} \right] \ln \left(\frac{A_S}{A_D} \right) + 2\dot{m}_A}{\left(\frac{\rho_D + \rho_{A0}}{2} \right) (A_S - A_D)} - U_D \cos \lambda \quad (4.43)$$

and A_{EFF} = effective surface area between "D" and "S" (m^2).

$$A_{EFF} = L_S \sqrt{\pi(A_S^{1/2} + A_D^{1/2})} \quad (4.44)$$

The expression for A_{EFF} assumes the region between the "D" plane and the "S" plane can be approximated by a conical volume.

Finally, the jet length between "D" and "S" (L_S) can be obtained by substituting Equations 4.42 to 4.44 into Equation 4.41 and solving for L_S with the known value of $\dot{m}_A$.

The elevation of the "S"-plane above the ground is:

$$Z_S = Z_E + L_S \sin \lambda \quad (4.45)$$

where Z_E = elevation of the rupture point "E" in Figure 4.2. Note that the length of the pressure equalization zone (L_Q) and drag zone (L_D) have been ignored since $L_S \gg L_Q$ or L_D .

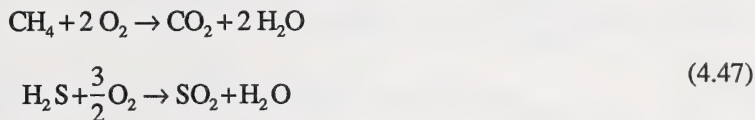
It is possible to specify M_S such that the velocity at "S" is greater than at "D" ($V_S > V_D$), which can only be obtained if mass is removed from the jet. To avoid this, the Mach number at the "D" plane is compared to M_S and if it is less ($M_D < M_S$), the above calculations are skipped and:

$$\begin{aligned} \dot{m}_S &= \dot{m}_D \\ T_S &= T_D \\ V_S &= V_D \\ A_S &= A_D \\ \rho_S &= \rho_D \end{aligned} \quad (4.46)$$

4.2.5 Combustion Zone

In the event that the gas-air mixture is ignited, as could be the case for an uncontrolled release of sour gas, the chemical transformation of the gas-air jet upon combustion and the increase in jet temperature due to the heat of combustion must be modelled.

Assuming the chief components of sour gas to be methane (CH₄), hydrogen sulphide (H₂S) and carbon dioxide (CO₂) and the components of air to be nitrogen (N₂ : 79% by volume; 76.8 % by mass) and oxygen (O₂ : 21% by volume; 23.2% by mass), the primary combustion reactions of interest are:



Complete combustion of H₂S and CH₄ is assumed in the region between "S" and "C" as shown in Figure 4.2, as excess air is provided.

The molecular mass of the combustible gas and air mixture at "C" depends on the mass flow of the various species at the "C" plane:

$$\frac{1}{M_{WC}} = \frac{(\dot{m}_C)_{\text{CO}_2}}{M_{W\text{CO}_2}\dot{m}_C} + \frac{(\dot{m}_C)_{\text{SO}_2}}{M_{W\text{SO}_2}\dot{m}_C} + \frac{(\dot{m}_C)_{\text{H}_2\text{O}}}{M_{W\text{H}_2\text{O}}\dot{m}_C} + \frac{(\dot{m}_C)_{\text{N}_2}}{M_{W\text{N}_2}\dot{m}_C} + \frac{(\dot{m}_C)_{\text{O}_2}}{M_{W\text{O}_2}\dot{m}_C} \quad (4.48)$$

where:

- $M_{W\text{CO}_2}$ = molecular mass of CO₂ = 44 kg/kmole
- $M_{W\text{SO}_2}$ = molecular mass of SO₂ = 64 kg/kmole
- $M_{W\text{H}_2\text{O}}$ = molecular mass of H₂O = 18 kg/kmole
- $M_{W\text{N}_2}$ = molecular mass of N₂ = 28 kg/kmole
- $M_{W\text{O}_2}$ = molecular mass of O₂ = 32 kg/kmole
- M_{WC} = molecular mass of combustible gas air mixture at "C" (kg/kmole)
- $\dot{m}_C$ = mass flow of combustible gas and air at "C" (kg/s)
- $(\dot{m}_C)_{\text{CO}_2}$ = mass flow of CO₂ at "C" (kg/s)
- $(\dot{m}_C)_{\text{SO}_2}$ = mass flow of SO₂ at "C" (kg/s)
- $(\dot{m}_C)_{\text{H}_2\text{O}}$ = mass flow of H₂O at "C" (kg/s)
- $(\dot{m}_C)_{\text{N}_2}$ = mass flow of N₂ at "C" (kg/s)
- $(\dot{m}_C)_{\text{O}_2}$ = mass flow of O₂ at "C" (kg/s)

The mass flows of the various species depend on the mass fractions of CH₄, H₂S and CO₂ in the sour gas at "S", the mass flow of sour gas at "S", the total mass flow (sour gas and air) at "S", and the mass flow of air entrained between "S" and "C":

$$(\dot{m}_C)_{CO_2} = a\dot{m}_E \frac{M_{WCO_2}}{M_{WCH_4}} + (1-a-b)\dot{m}_E \quad (4.49)$$

$$(\dot{m}_C)_{SO_2} = b\dot{m}_E \frac{M_{WSO_2}}{M_{WH_2S}} \quad (4.50)$$

$$(\dot{m}_C)_{H_2O} = 2a\dot{m}_E \frac{M_{WH_2O}}{M_{WCH_4}} + b\dot{m}_E \frac{M_{WH_2O}}{M_{WH_2S}} \quad (4.51)$$

$$(\dot{m}_C)_{N_2} = 0.768(\dot{m}_S - \dot{m}_E) + 0.768\dot{m}_{AC} \quad (4.52)$$

$$(\dot{m}_C)_{O_2} = 0.232(\dot{m}_S - \dot{m}_E) + 0.232\dot{m}_{AC} - 2a\dot{m}_E \frac{M_{WO_2}}{M_{WCH_4}} - \frac{3}{2}b\dot{m}_E \frac{M_{WO_2}}{M_{WH_2S}} \quad (4.53)$$

where:

a = mass fraction CH₄ in sour gas

$$= V_{CH_4} \frac{M_{WCH_4}}{M_{WE}} \quad (4.54)$$

b = mass fraction H₂S in sour gas

$$= V_{H_2S} \frac{M_{WH_2S}}{M_{WE}} \quad (4.55)$$

$(1-a-b)$ = mass fraction CO₂ in sour gas

$\dot{m}_{AC}$ = mass flow of air entrained between "S" and "C" (kg/s)

V_{H_2S} = volume fraction H₂S in the escaping gas

V_{CH_4} = volume fraction of CH₄ in the escaping gas.

Similarly, the relation for the specific heat at constant pressure at "C" is:

$$C_{PC} = \frac{(\dot{m}_C)_{CO_2}}{\dot{m}_C} C_{PCO_2} + \frac{(\dot{m}_C)_{SO_2}}{\dot{m}_C} C_{PSO_2} + \frac{(\dot{m}_C)_{H_2O}}{\dot{m}_C} C_{PH_2O} + \frac{(\dot{m}_C)_{N_2}}{\dot{m}_C} C_{PN_2} + \frac{(\dot{m}_C)_{O_2}}{\dot{m}_C} C_{PO_2} \quad (4.56)$$

where the specific heats at constant pressure (C_p) are dependent upon the temperature at "C" (T_C) (Himmelblau, 1974):

$$C_{p_{CO_2}} = \frac{4184}{44} [6.393 + 1.01 \cdot 10^{-2} T_C - 3.405 \cdot 10^{-6} T_C^2] \quad (4.57)$$

$$C_{p_{SO_2}} = \frac{4184}{64} [9.299 + 9.33 \cdot 10^{-3} (T_C - 273) - 7.418 \cdot 10^{-6} (T_C - 273)^2 + 2.057 \cdot 10^{-9} (T_C - 273)^3] \quad (4.58)$$

$$C_{p_{H_2O}} = \frac{4184}{18} [6.970 + 3.464 \cdot 10^{-3} T_C - 4.83 \cdot 10^{-7} T_C^2] \quad (4.59)$$

$$C_{p_{N_2}} = \frac{4184}{28} [6.529 + 1.488 \cdot 10^{-3} T_C - 2.271 \cdot 10^{-7} T_C^2] \quad (4.60)$$

$$C_{p_{O_2}} = \frac{4184}{32} [6.732 + 1.505 \cdot 10^{-3} T_C - 1.791 \cdot 10^{-7} T_C^2] \quad (4.61)$$

In the above equations, the specific heats at constant pressure are expressed in units of J/(kg K).

The properties of the combustible gas-air mixture at "C" depend on two unknown quantities: $\dot{m}_{AC}$ and T_C . The amount of air added is set to provide twice the amount of air required for stoichiometric combustion at the "C" plane (100% excess air). Air entrained in the jet at the "S" plane ($\dot{m}_s - \dot{m}_E$) is accounted for in determining $\dot{m}_{AC}$:

$$\dot{m}_{AC} = \frac{2\dot{m}_E}{.232} \left(2a \frac{M_{WO_2}}{M_{WCH_4}} + \frac{3}{2} b \frac{M_{WO_2}}{M_{WH_2S}} \right) - (\dot{m}_s - \dot{m}_E) \quad (4.62)$$

Providing 100% excess air is consistent with Brzustowski's (1973) buoyancy dominated flame model formulation used to estimate the flame length. The model uses the lean flammability limit C_L as a criteria. The lean limit is about one half the stoichiometric concentration and can be obtained by providing twice as much air than required for a stoichiometric mixture. Once $\dot{m}_{AC}$ is specified, the other parameters can be determined by application of the conservation laws in the region between "S" and "C" in Figure 4.2.

Conservation of mass dictates that:

$$\dot{m}_C = \dot{m}_s + \dot{m}_{AC} = \rho_C A_C V_C \quad (4.63)$$

where: ρ_C = density of the combustible gas air mixture at "C" (kg/m³)
 A_C = cross-sectional area of the plume at "C" (m²)
 V_C = velocity of the combustible gas air mixture at "C" (m/s).

The conservation of momentum provides another governing equation:

$$\dot{m}_s V_s + \dot{m}_{AC} U_s \cos \lambda = \dot{m}_c V_c \quad (4.64)$$

where: U_s = ambient wind speed at height "S" (m/s)
 λ = angle of jet with horizontal.

Conservation of energy gives:

$$\dot{m}_s C_{PS} T_s + \dot{m}_s \frac{V_s^2}{2} + Q_{HE} \left[\frac{\dot{m}_E}{\rho_{EO}} (1 - f_R) \right] + \dot{m}_{AC} C_{PA} T_{AO} = \dot{m}_c C_{PC} T_c + \dot{m}_c \frac{V_c^2}{2} \quad (4.65)$$

where: Q_{HE} = heat produced by the combustion reaction (J/m³)
 f_R = fraction of heat produced by combustion which is lost by radiation
= 0.25 (Alberta Environment, 1980)
 ρ_{EO} = density of sour gas at standard conditions of 15 °C and 101.3 kPa
(kg/m³) (Equation 4.2).

The heat produced by the combustion reaction Q_{HE} is given in terms of low heat values for the components of sour gas. Thus, when the low heat value for the escaping sour gas is multiplied by the volume flow rate of sour gas exiting the rupture at the standard conditions ($\dot{m}_E/\rho_{EO}$), the rate of heat input to the jet (in J/s) is obtained.

The ideal gas law gives the density at the "C" plane:

$$\rho_c = \frac{P_{AO}}{R_c T_c} \quad (4.66)$$

with R_c given by Equation 4.3.

The flame length L_c is estimated from the following correlation by Brzustowski (1973):

$$L_c = 2 \sqrt{\frac{A_s}{\pi}} \left\{ 2.96 \left(\frac{\rho_s}{\rho_{AO}} \right)^{1/3} (F_{RC})^{1/5} \left(\frac{\dot{m}_E}{\dot{m}_s} \right)^{3/5} \left[1 + \frac{M_{WA}}{M_{WE}} \left(\frac{1}{0.297 C_L} - 1 \right) \right]^{3/5} \right\} \quad (4.67)$$

where:

$$F_{RC} = \frac{V_s^2}{2g \sqrt{\frac{A_s}{\pi}}} \left(\frac{\rho_{AO}}{\rho_s} \right)^{1/2} \frac{C_{PA} T_{AO}}{\frac{\dot{m}_E Q_H}{\dot{m}_s \rho_{EO}} + C_{PS} (T_s - T_{AO})} \quad (4.68)$$

$$C_L = \left\{ \frac{V_{H_2S}}{(V_{H_2S} + V_{CH_4}) C_{L(H_2S)}} + \frac{V_{CH_4}}{(V_{H_2S} + V_{CH_4}) C_{L(CH_4)}} \right\}^{-1} \quad (4.69)$$

F_{RC} = Froude number with combustion

C_L = fuel concentration at the lean flammability limit, fraction by volume

$C_{L(H_2S)}$ = H_2S concentration at the lean flammability limit, fraction by volume (0.043)

$C_{L(CH_4)}$ = CH_4 concentration at the lean flammability limit, fraction by volume (0.050)

g = acceleration due to gravity (9.81 m/s^2).

A closed system of equations for all unknowns at the "C" plane for the ignited case has been formed. The solution procedure for this equation set is given in Table 4.3.

Finally, the elevation of the "C" plane above the rupture point is:

$$Z_C = Z_S + L_C \quad (4.70)$$

where: Z_C = elevation of the "C" plane in Figure 4.2

Note that the length of the flame L_C is assumed to have only a vertical component. This results in a change in the effective release angle from λ to λ_C :

$$\lambda_C = \tan^{-1} \left[\frac{(Z_S + L_C)}{L_S \cos \lambda} \right] \quad (4.71)$$

Table 4.3
Estimation of "C" Plane Parameters.

The procedure may be summarized as follows:

- (1) Determine $\dot{m}_{ac}$ (Equation 4.62).
- (2) Assume $T_C = T_{A0}$.
- (3) Calculate $\dot{m}_C$ since $\dot{m}_S$ is known (Equation 4.63).
- (4) Calculate V_C (Equation 4.64).
- (5) Calculate M_{WC} from Equation 4.48 knowing all the species mass flows (Equations 4.49 to 4.53).
- (6) Calculate R_C (Equation 4.3).
- (7) Calculate C_{PC} (Equation 4.56). The species mass flows are known from Equations 4.49 to 4.53 and T_C has been guessed in step 2.
- (8) Calculate a new T_C (Equation 4.65).
- (9) Repeat (7) using new T_C until T_C used in (7) approaches T_C from (8).
- (10) Calculate ρ_C (Equation 4.66).
- (11) Calculate A_C (Equation 4.63).
- (12) Calculate L_C (Equations 4.67 to 4.69).

4.3 Plume Rise Module

Once the expanded jet leaves ground level, the momentum and buoyancy of the jet will influence its rise until, at the point of final rise, atmospheric dispersion becomes the predominant transport mechanism. While momentum dominates immediately after jet expansion and jet-like behavior results, eventually buoyancy becomes an important factor and plume-like behavior results. Following the treatment of Wilson (1985), and consistent with the treatment of the jet expansion, this region of the flow is assumed to be quasi-steady.

The usual approach to modelling plume rise follows the analysis of Briggs (1984), who derived analytical expressions for plume rise assuming that the atmosphere is neutral or stable, that the "bent-over plume" assumption holds, and that the discharge is vertically upwards. Since these assumptions are not always valid to the case of sour gas releases from wells or pipelines, an alternative approach is to model the jet/plume by numerically solving the conservation equations of mass, momentum and energy as they apply to the discharged sour gas. This approach is more general than the analytical expressions for plume rise in that fewer simplifying assumptions are necessary. This approach, which has been called "integral modelling" of plumes and jets, has been employed successfully by Ooms (1972), Slawson *et al.* (1980), Schatzmann (1979), and will be used here. However, Briggs (1984) empirical correlations for limiting the final rise of momentum jets and buoyant plumes will be used.

4.3.1 Integral Plume Rise Model

Slawson *et al.* (1980) evaluated both analytical and integral (numerical) models of plume rise as they applied to the dispersion of the Great Canadian Oil Sands Plume. They recommended an integral model for modelling the plume rise and growth of that plume. The approach adopted by this study is similar to that given by Slawson *et al.* (1980). Unlike the Slawson *et al.* approach however, this study accounts for plume "scuffing" on the ground for near horizontal releases (f_E/f_A terms) and employs different criteria for determining when the plume rise has to be terminated.

The governing conservation equations of the jet/plume may be derived from a control volume analysis of a section of the plume. The coupled set of first order ordinary differential equations for the conservation of mass, horizontal momentum, vertical momentum, energy and the concentration of a scalar (respectively) are:

$$\frac{d}{dt}(r^2 V \rho) = 2 \rho_A r V V_\alpha \left(\frac{f_E}{f_A} \right) \quad (4.72)$$

$$\frac{d}{dt}(r^2 V V_x \rho) = \left(\frac{f_E}{f_A} \right) [2 \rho_A r U V V_\alpha + \rho_A C_M r V (U - V_x) V_R] - \rho r V V_F^2 C_F \frac{\sin[\pi(1 - f_E)]}{f_A} \quad (4.73)$$

$$\frac{d}{dt}(r^2 V V_z \rho) = g r^2 V (\rho_A - \rho) - \rho_A C_M V V_z V_R r \left(\frac{f_E}{f_A} \right) \quad (4.74)$$

$$\frac{d}{dt} \left[r^2 V \rho \left(\frac{\theta - \theta_A}{\theta_A} \right) \right] = - \frac{\rho r^2 V V_z}{\theta_A} \left(\frac{d\theta_A}{dz} \right) \left(\frac{\theta}{\theta_A} \right) \quad (4.75)$$

$$\frac{d}{dt}(r^2 V C) = 0 \quad (4.76)$$

where: t = time (s)

r = plume radius (m)

$$\begin{aligned} V &= \text{plume velocity (m/s)} \\ &= \frac{ds}{dt} = \sqrt{V_x^2 + V_z^2} \end{aligned} \quad (4.77)$$

s = plume centreline coordinate (m)

$$\begin{aligned} V_x &= \text{horizontal velocity component of plume (m/s)} \\ &= \frac{dx}{dt} \end{aligned} \quad (4.78)$$

x = horizontal coordinate (m)

$$V_z = \text{vertical velocity component of plume (m/s)} \quad (4.79)$$

$$= \frac{dz}{dt}$$

f_E = factor to account for plume circumferential area reduction due to ground impingement ($f_E = 1$ for elevated plumes)

f_A = factor to account for plume cross-sectional area reduction due to ground impingement ($f_A = 1$ for elevated plumes)

z = vertical coordinate (m)

ρ = density of plume (kg/m³)

ρ_{AO} = ambient air density (kg/m³)

$$= \rho_{AO} \exp \left[- \frac{\left(R_A \left(\frac{dT_A}{dz} \right) + g \right)}{R_A \left(\frac{dT_A}{dz} \right)} \ln \left(\frac{1 + \left(\frac{dT_A}{dz} \right) Z}{T_{AO}} \right) \right] \quad (4.80)$$

ρ_{AO} = ambient air surface density (kg/m³) (Equation 4.42)

V_α = entrainment velocity, for parameterizing the amount of ambient air which is entrained into the plume (m/s)

U = ambient wind speed (varies with z , Equation 3.29) (m/s)

$$V_R = \text{relative velocity between plume and atmosphere (m/s)} \quad (4.81)$$

$$= \sqrt{(V_x - U)^2 + V_z^2}$$

C_M = added mass factor to account for apparent additional mass of plume (set to 0.0 for tests)

V_F = relative velocity between plume and ground (m/s)

$$= \text{MAX}[0, V_x - U] \text{ for } V_x \geq 0 \quad (4.82)$$

$$= V_x \text{ for } V_x < 0$$

C_F = skin friction coefficient of plume impinging on ground (= 0.005)

θ = potential temperature of plume (varies with z) (K)

$$= T + \frac{g}{C_P} Z \quad (4.83)$$

T = plume temperature (K)

C_P = specific heat at constant pressure for the plume (J/(kg K))

g = acceleration of gravity (= 9.81 m/s²)

θ_A = potential temperature of atmosphere (K) (4.84)

$$= T_A + \frac{g}{C_{PA}} Z$$

C_{PA} = specific heat at constant pressure of ambient air (1005 J/(kg K))

T_A = ambient temperature (K)

$$= T_{A0} + \left(\frac{dT_A}{dZ} \right) Z \quad (4.85)$$

T_{A0} = ambient surface temperature (K)

$\frac{dT_A}{dZ}$ = vertical temperature gradient in atmosphere for given stability (K/m)

$\frac{d\theta_A}{dZ}$ = potential temperature gradient of atmosphere (K/m)

$$= \frac{g}{C_{PA}} + \frac{dT_A}{dZ} \quad (4.86)$$

c = concentration of scalar species (e.g., H₂S) in the plume (kg/m³).

In order to form a closed equation set for the dependent variables ρ , V , V_x , V_z , r , θ , c , s , z and x , it remains to specify five additional independent equations;

$$\frac{d}{dt}(\rho T) = \frac{-\rho_A g V_z}{R} \quad (4.87)$$

$$\frac{ds}{dt} = V \quad (4.88)$$

$$\frac{dz}{dt} = V_z \quad (4.89)$$

$$\frac{dx}{dt} = V_x \quad (4.90)$$

$$\frac{dV}{dt} = \frac{V_x}{V} \frac{dV_x}{dt} + \frac{V_z}{V} \frac{dV_z}{dt} \quad (4.91)$$

where R is the gas constant for plume (J/kg K). The first of these additional five equations is the hydrostatic pressure law; the last four are kinematic relationships for the plume trajectory. It should be noted that, in the derivation of the above conservation equations, "top hat" profiles (i.e., uniform in the plume cross-section) have been assumed for all the independent plume variables.

Ambient temperature, density and pressure vary with the plume elevation depending on the atmospheric stability. The user must input ambient surface temperature and pressure and has the option to provide the vertical temperature gradient for the atmospheric stability being considered. Default values of the vertical temperature gradient dT_A/dZ (K/m) are:

$$\text{Unstable} = -0.0148 \quad (4.92)$$

$$\text{Neutral} = -0.0098$$

$$\text{Stable} = +0.0302$$

The concept behind the "scuffing" of the plume on the ground for near horizontal releases is illustrated in Figure 4.3. The factor f_E appearing in the governing differential equations is an "entrainment" factor which accounts for the decrease in the circumferential surface area of the plume which is available for air entrainment when the ground "removes" the lower portion of the plume. The plume is assumed to have a circular cross-section.

The f_E factor is a function of plume radius and height of the plume centreline above the ground:

$$f_E = 1 - \frac{1}{\pi} \cos^{-1} \left(1 - \frac{\delta}{r} \right) \quad (4.93)$$

where:

$$\delta = \text{MAX} \left[r - \frac{z}{\cos \phi}, 0 \right] \quad (4.94)$$

$$\phi = \tan^{-1} \left(\frac{V_z}{V_x} \right) \quad (4.95)$$

The factor f_A appearing in the governing differential equations is a "cross-sectional area" factor which accounts for the decrease in the cross-sectional area of the plume when the ground "removes" the lower portion of the plume. The f_A factor is given by:

$$f_A = f_E + \frac{r(r - \delta)}{\pi r^2} \sin[\pi(1 - f_E)] \quad (4.96)$$

Again, this factor depends on the radius of the plume and the height of the plume centreline above the ground.

The ratio (f_E/f_A) is of primary importance for horizontal plumes in the governing differential equations. This is because the growth rate of the plume will increase if the reduction in the air entrainment is smaller than the ability of the plume to transport mass through its cross section.

The last term on the right hand side of Equation 4.73 (the C_F term) accounts for the skin friction drag experienced by a plume as it scuffs across the ground. The drag is only allowed to act if the horizontal plume velocity exceeds the local wind speed or the plume has a negative horizontal velocity. This is because the local wind speed derived from the power law wind speed profile already accounts for ground shear and it is this momentum that is entrained into the plume. The area over which the skin friction drag acts is the intersection area of the circular plume and the ground.

The added mass factor C_M is included to allow for the apparent additional mass of the plume due to the air which has been displaced. Plume rise and spread is reduced as C_M is increased from a value of zero. Better agreement between model trajectory predictions and observations have been noted by several researchers (Slawson (1980), Davidson (1988), and Schatzmann (1979)) with C_M values of the order of 0.5.

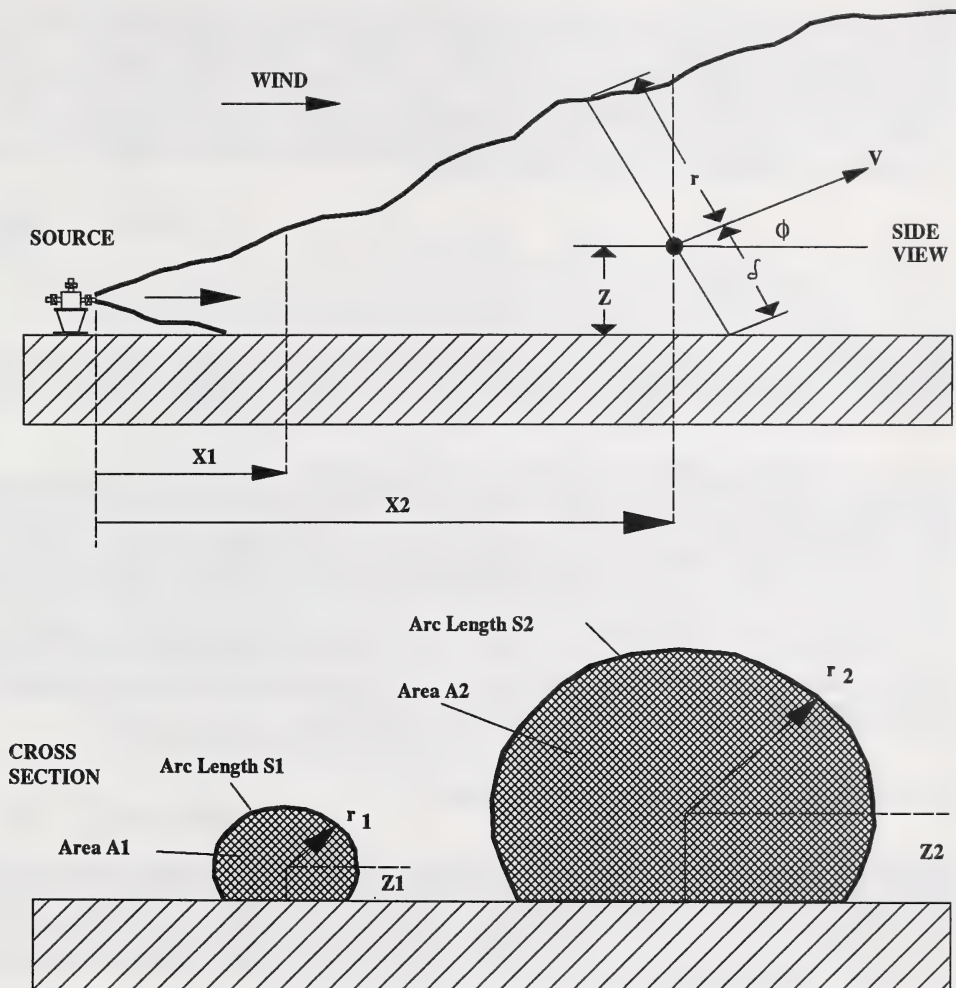


Figure 4.3
Plume Scuffing for a Horizontal Plume.

The equation set for the ten independent variables is closed if the entrainment velocity V_α is specified as a function of previously defined variables. The entrainment velocity is an extremely important parameter which influences the spread of the plume. There have been many different forms for V_α suggested in the literature. A summary of various entrainment models may be found in Gebhart *et al.* (1984). The formulation used in this model has been suggested by Abraham (1971) and Ooms (1972):

$$V_\alpha = \alpha \left| V - \frac{UV_x}{V} \right| + \beta \frac{|V_x|}{V} \left| \frac{UV_z}{V} \right| \quad (4.97)$$

with $\alpha \sim 0.13$ and $\beta \sim 0.58$. This form has been recommended by Slawson *et al.* (1980) and possesses the desirable property that the correct limiting forms are recovered for vertical jet entrainment near the source and bent-over plume entrainment further away.

Finally, it can be stated that the system described in this section represents a closed equation set for the variables ρ , r , V , V_x , V_z , θ , c , z , x , and s . The equations for these variables, which are coupled and non-linear, are solved by using the Livermore Solver for Ordinary Differential Equations with General Jacobian Matrices ("LSODES") (Hindmarsh, 1980), given initial values (i.e., at time $t = 0$) for the variables. The required initial values are known after the jet expansion stage of the sour gas release, as negligible time is assumed to have elapsed from the onset of the gas release. Furthermore, since transient "storage" terms have been neglected in the derivation of the conservation equations, the jet/plume is assumed to adjust instantaneously to changes in source conditions.

4.3.2 Integral Plume Rise Termination

The numerical integration of the governing differential equations of the jet/plume yield, as part of the solution, the trajectory (z versus x) of the plume centreline. It remains to specify criteria for terminating the numerical integration once the "final rise" has occurred. The criteria to terminate integral plume rise calculations are summarized below in the order they are tested. The letter corresponds to the flag printed on output.

(a) Height

In neutral and unstable boundary layers, Slawson *et al.* (1980) suggest terminating the integral plume rise model when the plume elevation exceeds that predicted by the (standard) Briggs plume rise relations. This approach seems prudent in that the plume rise attained by the integral model is never allowed to deviate significantly from the Briggs prediction while the integral model is permitted to predict the initial dilution and downwind displacement of the plume.

Briggs plume rise estimates are employed as a termination criteria. The calculation of Briggs plume rise estimates for boundary layers of unstable, neutral or stable stability is presented in Section 4.3.3. The Briggs final plume elevation is denoted by $Z_{PF, BRIGGS}$.

If the Briggs' final rise estimate $Z_{PF, BRIGGS}$ is sufficiently greater than the mixed layer height, then plume penetration will occur according to the plume penetration model described in Section 4.5.1. In this event, a better estimate of the final plume elevation is some elevation ($Z_{PF, PEN}$) less than or equal to the mixed layer height. Hence, it is more appropriate to terminate the integral plume rise model when the plume elevation Z_P exceeds $Z_{PF, MAX} = \text{MIN} [Z_{PF, BRIGGS}, Z_{PF, PEN}]$.

(b) **Velocity**

For stable boundary layers, the predicted trajectory will oscillate and reach a maximum elevation when the vertical component of plume velocity is equal to zero ($V_z = 0$). The plume height then decreases ($V_z < 0$) to a minimum value. Integral plume rise is terminated at this point, where $V_z = 0$ for a second time. Final plume rise $Z_{PF, MAX}$ is set at the average of the two elevations where $V_z = 0$.

For neutral and unstable conditions, if the plume speed is sufficiently slow, then it is advisable to terminate the integral plume rise to save computational effort and to reduce the downwind displacement at which the calculation of ground-level concentrations may begin. If the relative velocity is less than 5% of the wind speed, the integral plume rise calculations terminate.

(c) **Downwind Position**

This criterion is based on the downwind position of the plume exceeding 500 m and was adapted to save computational effort.

(d) **Dense Gases**

For dense gases where the buoyancy flux is negative, the plume height is allowed to decrease until only 1 metre of the scuffed radius is above the ground. When $Z_F + R_F$ is less than 1.0 m, termination occurs.

Trajectory

If plume rise termination occurs at the " $Z_{PF, MAX}$ " criteria, then the plume elevation is deemed to be at the maximum permissible value and the passive dispersion formulations employ a constant plume elevation at the value where the rise is terminated. If plume terminates at some **earlier** criterion, then the plume must be allowed to rise further to its maximum permissible elevation. To accomplish this, the plume elevation is allowed to track the following trajectory:

$$Z_P = \left[\frac{3F_M}{\beta^2 U_P^2 (1 + C_M)} x_s + \frac{3F_B}{2\beta^2 U_P^3 (1 + C_M)} x_s^2 + \left(\frac{r_o}{\beta} \right)^3 \right]^{1/3} - \frac{r_o}{\beta} + Z_s \quad (4.98)$$

where:

F_M = momentum flux defined in Table 4.6 (m^4/s^2)

F_B = buoyancy flux defined in Table 4.6 (m^4/s^3)

U_P = wind speed at plume height (m/s)

C_M = added mass factor

r_O = equivalent radius for virtual origin correction (m)

$$= r_S \sqrt{\frac{V_{SZ} \rho_S}{U_P \rho_{AO}}} \quad (4.99)$$

V_{SZ} = vertical component of velocity at "S" plane or "C" plane (m/s)

r_S = plume radius at the "S" plane or "C" plane (m)

β = entrainment constant = 0.58

Z_P = plume elevation (m)

x_S = virtual distance (m)

$$= x - x_F + x_V$$

x = downwind distance from rupture point (m)

x_F = downwind distance from rupture point when integral plume rise model is terminated (m)

x_V = distance calculated by forcing the derivative of the above equation for Z_P to equal the angle of travel (V_Z / V_X) when the integral plume rise model is terminated at $x = x_F$ (m)

Z_S = elevation of "S" or "C" plane above the ground (m).

Equation 4.98 for Z_P is the solution to the plume equations (Equations 4.72 to 4.76) with the following restrictions:

- (1) Vertical discharge ($\lambda = 90^\circ$)
- (2) Neutral stability ($d\theta_A/dz = 0$)
- (3) Bent-over plume ($V_X \sim U_P$)
- (4) Constant wind speed with elevation ($U_P = \text{constant}$)
- (5) Bent-over plume entrainment ($V_\alpha = \beta |V_Z|$)
- (6) No added mass factor ($C_M = 0$)
- (7) Boussinesq approximation ($\rho = \rho_A$, except in buoyancy terms)

The application of Equation 4.98 for Z_P continues for downwind distances as long as the maximum permissible plume elevation is not exceeded. Once the maximum elevation is attained, the plume height is considered constant at that value further downwind.

4.3.3 Briggs' Final Plume Rise Estimates

Briggs' expressions for the final plume rise in unstable, neutral and stable atmospheres are used to arrive at the Briggs' final plume elevation $Z_{PF, BRIGGS}$. Definitions for buoyancy and momentum fluxes are given in Table 4.4.

Unstable and Neutral Atmospheres

The Ontario Ministry of the Environment (OME) (1986) has recommended the use of Briggs' (1984) expression for the final buoyancy rise in unstable conditions:

$$(\Delta h_B)_U = 3.0 Z_i \left(\frac{F_B}{W^{*2} U_P Z_i} \right)^{0.6} \quad (4.100)$$

W^* = convective velocity scale from Equation 3.18 (m/s)

Z_i = mixed layer depth (m)

U_P = wind speed at plume height (m/s)

The terminal rise due to buoyancy in a neutral boundary layer may be approximated as (Briggs, 1975):

$$(\Delta h_B)_N = \frac{1.3 F_B}{U_P U^{*2}} \left(1 + \frac{Z_S}{(\Delta h_B)_N} \right)^{2/3} \quad (4.101)$$

where Z_S = initial height of the source at the "S" plane of Figure 4.2 (or the "C" plane if there is ignition) (m).

The final momentum rise for both unstable and neutral conditions can be estimated from (Briggs, 1975):

$$\Delta h_M = 1.5 \left(\frac{F_M}{U_P U^*} \right)^{1/2} \quad (4.102)$$

where U^* = surface friction velocity (m/s).

Table 4.4
Buoyancy (F_B) and Momentum (F_M) Fluxes.

The buoyancy flux and momentum flux are defined as follows:

$$F_B = g V_s r_s^2 \left(\frac{\rho_{AO} - \rho_s}{\rho_{AO}} \right) \quad (\text{m}^4/\text{s}^3) \quad (4.103)$$

$$F_M = \frac{\rho_s}{\rho_{AO}} V_s V_{SZ} r_s^2 \quad (\text{m}^4/\text{s}^2) \quad (4.104)$$

where:

- ρ_{AO} = ambient air density at ground level (kg/m^3)
- g = acceleration of gravity ($9.81 \text{ m}/\text{s}^2$)
- ρ_s = density of gas effluent at the source (kg/m^3)
- r_s = radius of effluent jet at the source (m)
- V_s = velocity of effluent jet at the source (m/s)
- V_{SZ} = vertical component of V_s (m/s)
 $= V_s \sin \lambda$
- λ = angle of effluent release at source
(with respect to the horizontal).

Note that the source parameters (ρ_s , r_s and V_s) refer to the conditions at the "S" plane for the nonignited case and the conditions at the "C" plane for the ignited case (Figure 4.2).

For very low wind speed values (as U_p approaches zero), the predicted plume rise increases rapidly (approaching infinity). The Briggs plume rise relationships for unstable and neutral conditions do not account for these near calm conditions. It is for this reason that a stable plume rise relationship applicable to near calm conditions is evaluated for low wind speed conditions:

$$\Delta h_{SC} = 5.0 \frac{F_B^{1/4}}{S^{3/8}} \quad (4.105)$$

where the stability parameter S (s^{-2}) is given by:

$$S \equiv \frac{g}{\theta_A} \left(\frac{\partial \theta_A}{\partial Z} \right) = \frac{g}{T_A + \frac{dT_A}{dZ} Z_{SC}} \left(\frac{dT_A}{dZ} + \gamma_D \right) \quad (4.106)$$

where:

g = acceleration due to gravity (9.81 m/s^2)

θ_A = potential temperature (K)

$\partial \theta_A / \partial Z$ = potential temperature gradient (K/m)

$Z_{SC} = Z_s + \Delta h_{SC}$

dT_A/dZ = average vertical temperature gradient in the atmosphere
= -0.0065 K/m (e.g., Briggs, 1969)

T_{A0} = ambient surface temperature (K)

γ_D = dry adiabatic lapse rate (0.0098 K/m).

The combined effect of buoyancy and momentum rise may be estimated using the "sum-of-cubes" formula recommended by Wilson (1986). Two final rises are calculated:

$$\Delta h_1 = \left[\Delta h_M^3 + \Delta h_B^3 + \left(\frac{r_O}{\beta} \right)^3 \right]^{1/3} - \frac{r_O}{\beta} \quad (4.107)$$

$$\Delta h_2 = \left[\Delta h_M^3 + \Delta h_{SC}^3 + \left(\frac{r_O}{\beta} \right)^3 \right]^{1/3} - \frac{r_O}{\beta} \quad (4.108)$$

where β = entrainment constant = 0.58, and r_O is given by Equation 4.99.

Three cases need to be considered to arrive at the final Briggs plume rise value for unstable or neutral conditions (Δh):

- (a) If plume height ($Z_s + \Delta h_1$) is greater than Z_i and ($Z_s + \Delta h_2$) is less than Z_i , then $\Delta h = Z_i - Z_s$. That is, the plume height is limited by the inversion height.
- (b) If both plume heights [$(Z_s + \Delta h_1)$ and $(Z_s + \Delta h_2)$] are greater than Z_i , then $\Delta h = \text{MIN}(\Delta h_1, \Delta h_2)$. That is, the plume is assumed to penetrate the inversion height.
- (c) If the plume height ($Z_s + \Delta h_1$) is less than Z_i , then $\Delta h = \Delta h_1$. The plume remains in the mixing layer.

where Z_s = initial height of the source at the "S" plane of Figure 4.2 (or the "C" plane if there is ignition) (m) and Z_i is the depth of the mixing layer. The letter corresponds to the flag printed on output.

Finally, $Z_{PF, BRIGGS} = Z_s + \Delta h$.

Stable Atmospheres

The final buoyancy rise in a stable atmosphere may be estimated from the following expression (Briggs, 1975):

$$(\Delta h_B)_s = 2.6 \left(\frac{F_B}{U_p S_o} \right)^{1/3} \quad (4.109)$$

where S_o = the square of the Brunt-Vaisala frequency (s^{-2})

$$S_o = \frac{U^{*2}(0.74 + 4.7Z_M/L)}{k^2 L Z_M} \quad (4.110)$$

where: k = von Karman constant (= 0.40)
 Z_M = MAX[1, MIN(Z_s , $2L$)] (m)
 L = Monin-Obukhov length (m).

Equation 4.110 is obtained by substituting the surface similarity values for θ_A and $\partial\theta_A/\partial Z$ into the definition for S (Equation 4.106) (e.g., OME, 1986). According to the above definition, Z_M is not allowed to be less than 1 m or more than the minimum of Z_s or $2L$. A typical minimum value for $2L$ is 40 m (Table 3.4).

For very low wind speed conditions (calms), estimates of the buoyancy plume rise can also be obtained from:

$$(\Delta h_B)_{SC} = 5.0 \frac{F_B^{1/4}}{S^{3/8}} \quad (4.111)$$

where S is given by Equation 4.106.

For stable conditions, this study adopts:

$$\Delta h_B = \text{MIN}[(\Delta h_B)_S, (\Delta h_B)_{SC}] \quad (4.112)$$

The final momentum rise may be approximated using Briggs (1969):

$$\Delta h_M = 1.5 \left(\frac{F_M}{U_P S_O^{1/2}} \right)^{1/3} \quad (4.113)$$

The combined effect of buoyancy and momentum rise is estimated using the "sum-of-cubes" formula recommended by Briggs (1975);

$$\Delta h = \left[\Delta h_M^3 + \Delta h_B^3 + \left(\frac{r_O}{\beta} \right)^3 \right]^{1/3} - \frac{r_O}{\beta} \quad (4.114)$$

where β = entrainment constant = 0.58, and r_O is given by Equation 4.99.

Finally, $Z_{PF, BRIGGS} = Z_S + \Delta h$.

4.3.4 Accounting for Wind Speed Shear in Plume Rise

The calculation of plume rise from the integral plume model and from the Briggs plume rise relationships are dependent on the wind speed at plume height (Z_p). Plume height, of course, is not known until the plume rise is known. Therefore, the calculation of the plume rise Δh is iterative in nature. This iteration can proceed as follows:

- (1) Let $U_p = U_{REF}$ (the wind speed at anemometer height Z_{REF} , usually 10 m).
- (2) Calculate the plume rise Δh .
- (3) Calculate a new value of U_p at $Z = Z_p + \Delta h$ using the Irwin power law wind profile relationship (Equation 3.29). The wind speed U_p can never exceed the wind speed at 100 m or be less than the wind speed at 1 m.
- (4) Go back to (2) and recalculate Δh .
- (5) If Δh has converged to a value within 1 percent, then the iteration can be stopped. If the difference between the previous and the current estimates is greater than 1 percent, keep modifying Δh and U_p until these values converge. To reduce computational resources, no more than 15 iterations are allowed.

Normally, the height of the plume (Z_p) is greater than the reference wind speed height (Z_{REF}). Based on Equation 3.29, it follows that the wind speed at Z_p will be greater than the wind speed at Z_{REF} . The use of the larger wind speed value at Z_p in the previously discussed plume rise formulations will produce smaller plume rise values.

4.4 Transient Release Module

Releases of toxic gas from a pipeline or a pressure vessel rupture are characterized by a time varying mass discharge rate of gas. The mass emission module used in this model for a pipeline rupture has been described in Section 4.1.2.

The steady-state plume dispersion equations ignore diffusion in the along wind direction. For a transient release, the along wind diffusion cannot be ignored and can be accounted for by either of the following methods:

- An integrated puff model which superimposes a series of individual puffs (Section 5.7.5).
- An effective mass correction which allows the use of the steady state dispersion equation (Wilson, 1979).

The first method requires considerable computer resources to superimpose the puffs. For this reason, the second method was adopted for this project.

A basic assumption in the transient module is that the rise of the effluent gas jet and plume is determined by the instantaneous mass emission rate. This means that for any downwind distance x from the rupture, the mass rate that determines the plume elevation at that distance and time is:

$$\dot{m}_E(\tau) \quad \text{where} \quad \tau = t - \frac{x}{\bar{U}} \quad (4.115)$$

where the transient mass rate $\dot{m}_E$ is a function of time after release as described in Section 4.1.2 and $\bar{U}$ is the mean transport wind speed of the plume. This procedure is the same as employed by Wilson (1979) where the above equation is referred to as the "frozen mass rate" (Figure 4.4). The physical justification of using a frozen mass rate rather than the effective mass rate (see below) is that plume rise is related to vertical movement and along-wind diffusion will not alter the trajectory of the centre of mass to any significant extent.

The transient release module first calculates plume rise from the rupture point to the distance downwind where passive dispersion takes over the plume transport (X_F) for a number of frozen mass rates beginning with $\dot{m}_E(0)$ (the initial mass rate) and ending with MAX $[(\dot{m}_{E,S}, \dot{m}_E(t_E))]$ (the maximum of a user specified steady mass rate or the flow rate at t_E when 99% of the gas has been released). A user specified number of increments between these two frozen mass rate limits are used to construct a table of frozen mass rate versus plume parameters such as:

- Plume elevation, radius and temperature at downwind distance X_F ,
- Penetration fraction, and
- Final plume elevation.

Two important notes need to be mentioned regarding the evaluation of frozen mass rate. First, the mean transport wind speed $\bar{U}$ is evaluated as:

$$\bar{U} = U_{REF} \quad (4.116)$$

Second, for lagged time $(t - x/\bar{U})$ less than zero, it is not clear what the frozen mass rate should be. In this model, the conservative assumption is made:

$$\begin{aligned} \dot{m}_E &= \dot{m}_E(0) & \text{for} & \quad \tau < 0 \\ &= \dot{m}_E(\tau) & \text{for} & \quad \tau \geq 0 \end{aligned} \quad (4.117)$$

In order to account for along-wind diffusion of the transient sources, the "effective mass flux" concept of Wilson (1981) which accounts for along wind dispersion (Figure 4.4) is employed.

$$\dot{m}_{EFF}(x_1, t) = \int_{x=-\infty}^{x=\bar{U}t} \frac{\dot{m}_E(\tau)}{\sqrt{2\pi}\sigma_{x_1}} \exp\left[-\frac{(x_1 - x)^2}{2\sigma_{x_1}^2}\right] dx \quad (4.118)$$

where $\dot{m}_E(\tau)$ is given by the double exponential blowdown relationship (Equation 4.4) and:

$$\sigma_{x_1} = \left[0.09 \left(\frac{n x_1}{Z_R} \left(\frac{Z_R}{Z_V} \right)^n \right)^2 + \alpha_2 \right]^{1/2} \sigma_Z \quad (4.119)$$

where:

σ_{x_1} = standard deviation of the transient plume in the along wind direction at downwind distance X_1 (m).

σ_Z = standard deviation of the transient plume in the vertical direction at downwind distance X_1 (m).

$$\begin{aligned} Z_R &= Z_P + 0.5\sigma_Z & (4.120) \\ &= \text{reference height at which effective wind shear is evaluated (m).} \end{aligned}$$

$$\begin{aligned} Z_V &= Z_P + 0.17\sigma_Z & (4.121) \\ &= \text{reference height at which wind speed equals convection speed (m)} \end{aligned}$$

n = velocity profile power law exponent (Irwin model) (Table 3.5)

α_2 = a stability dependent constant (6.0 for unstable, 8.0 for neutral and 10.0 for stable).

The "effective mass" $\dot{m}_{EFF}$ multiplied by the mass fraction of H_2S is the release rate used in the dispersion relationships to estimate the ground level concentrations as a function of downwind distance and time for transient releases. Figure 4.5 illustrates that the effective mass is a function of time after the rupture and the downwind distance. A transient run involves the calculation of many effective mass rates using the method given in Table 4.5.

Table 4.5
Analytical Expression for the Effective Mass Release Rate.

The integral expression for the effective mass release rate is computed as the sum of three terms:

$$\dot{m}_{EFF}(x_1, t) = I_1 + I_2 + I_3 \quad (4.122)$$

The first and second terms account for the transient component of the mass release and the third term accounts for the steady-state component which may follow the transient portion. The transient release terms account for each exponential term in the double exponential blowdown model (Equation 4.5). The third term accounts for any steady-state release which may occur after time t_s as defined in Equation 4.13.

The term I_1 represents the integration from $x = -\infty$ to $t\bar{U}$ of the initial rapid decay transient (first term in Equation 4.5):

$$I_1 = \frac{\Gamma \dot{m}_o}{2(1+\eta)} \exp \left[-\left(\frac{1}{\eta^2 \epsilon} \right) \left(t - \frac{x_1}{\bar{U}} \right) \right] \exp \left[\frac{\sigma_{x_1}^2}{2\bar{U}^2 \eta^4 \epsilon^2} \right] \left[\operatorname{erfc} \left(\frac{\sigma_{x_1}}{\sqrt{2}\bar{U}\eta^2\epsilon} + \frac{x_1 - t\bar{U}}{\sqrt{2}\sigma_{x_1}} \right) \right] \quad (4.123)$$

The term I_2 also represents the integration from $x = -\infty$ to $t\bar{U}$ of the final slow decay transient (second term in Equation 4.5):

$$I_2 = \frac{\eta \Gamma \dot{m}_o}{2(1+\eta)} \exp \left[-\left(\frac{1}{\epsilon} \right) \left(t - \frac{x_1}{\bar{U}} \right) \right] \exp \left[\frac{\sigma_{x_1}^2}{2\bar{U}^2 \epsilon^2} \right] \left[\operatorname{erfc} \left(\frac{\sigma_{x_1}}{\sqrt{2}\bar{U}\epsilon} + \frac{x_1 - t\bar{U}}{\sqrt{2}\sigma_{x_1}} \right) \right] \quad (4.124)$$

The term I_3 represents the steady state component which may occur after time t_s :

$$I_3 = \frac{\dot{m}_{E,S}}{2} \left[\operatorname{erfc} \left(\frac{x_1 - (t - t_s)\bar{U}}{\sqrt{2}\sigma_{x_1}} \right) \right] \quad (4.125)$$

MASS RELEASE RATE

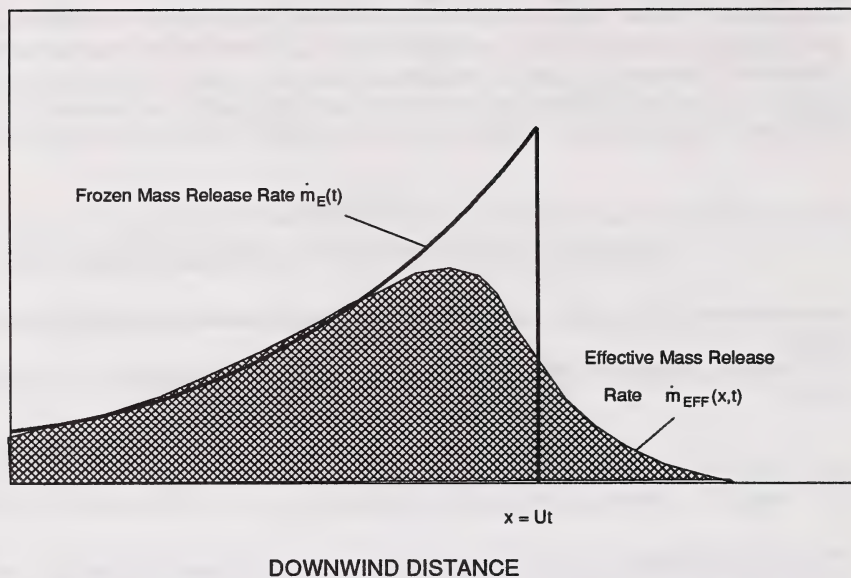


Figure 4.4

Comparison of the "Frozen" and "Effective" Mass Release Rates.

MASS RELEASE RATE

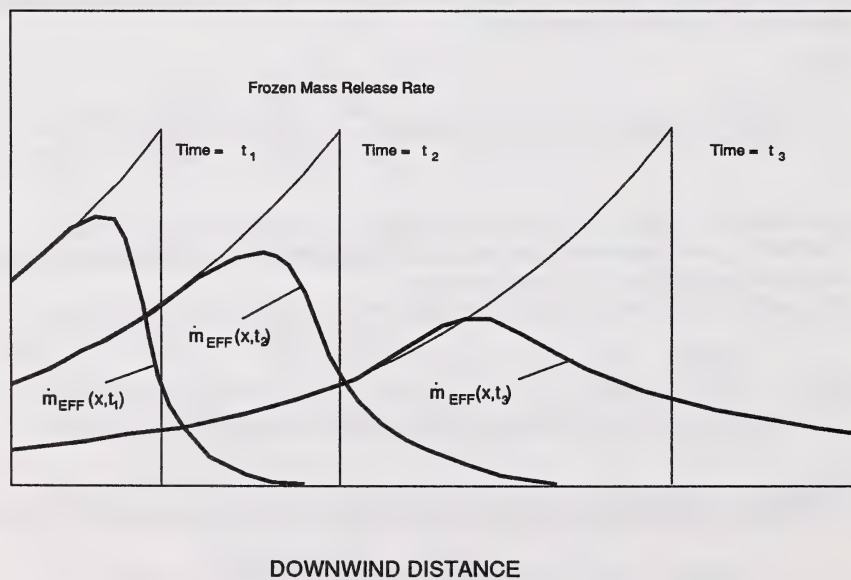


Figure 4.5

Frozen and Effective Mass Release Rates for Selected Times after the Rupture.

4.5 Passive Dispersion Module

During the jet expansion stage of a sour gas release, the behavior of the jet itself determines the initial trajectory and dilution of the plume; the turbulent behavior of the atmosphere is of secondary importance during this stage. At the completion of the jet dominated stage, the mean motion and turbulence of the atmosphere begin to dominate plume dispersion processes.

The ability of the atmosphere to disperse a plume is dependent on the level of turbulence in the atmosphere and on the presence of physical boundaries which restrict plume spread. Typical boundaries include the top of the mixed layer (upper boundary) and the ground (lower boundary). The relative location of the plume (after reaching final rise) with respect to these two boundaries is important in determining the dilution of the plume. Figure 4.6 illustrates three possible plume-boundary combinations:

- The plume is located very near or above the top of the mixed layer. The plume rise may, in certain conditions, be sufficient to allow the plume to penetrate the mixed layer. When this occurs, the downwind concentrations of plume gases will be reduced.
- The plume is elevated. This condition is most frequently assumed in the prediction of plume concentrations resulting from industrial stacks. The plume is usually assumed to have a Gaussian shape in both the vertical and the lateral directions.
- The plume is located near the surface. Due to limited plume rise, the plume remains sufficiently near the surface that the presence of the ground results in a non-Gaussian shape in the vertical direction.

The following discussion considers these three plume-boundary condition combinations with respect to unstable, neutral and stable atmospheres in the prediction of ground level plume concentrations.

4.5.1 Plume Penetration of the Mixed Layer

The fraction f is used to modify the mass flow $\dot{m}_p$ appearing in the passive dispersion parameterizations. The fraction of plume remaining in the mixed layer (f) for elevated releases is given in the following sections. Surface releases are not allowed to penetrate the mixed layer, thus $f = 1.0$.

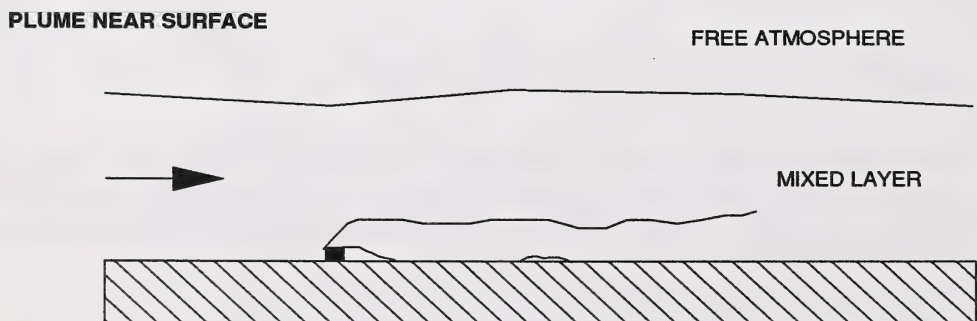
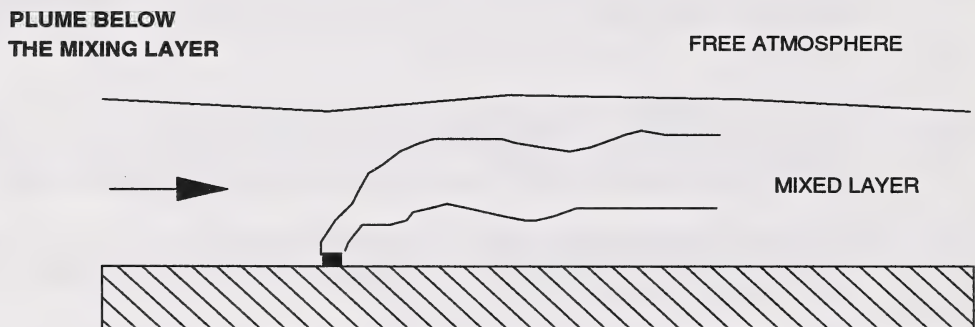
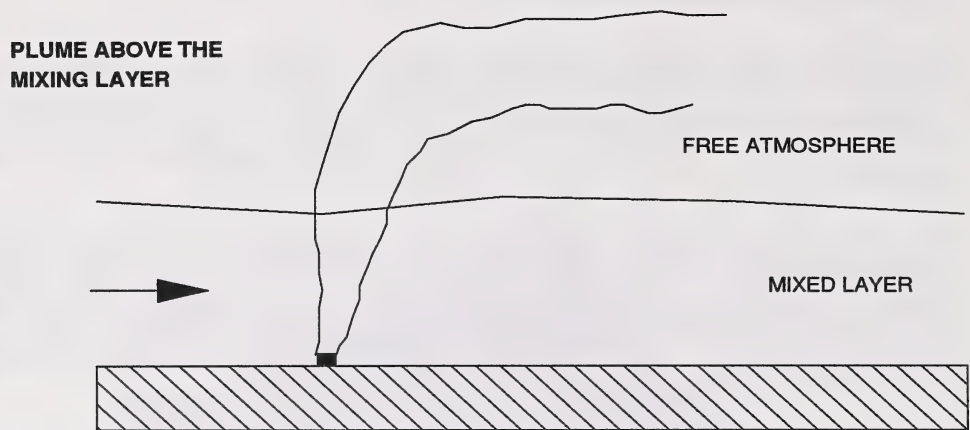


Figure 4.6
Three Possible Plume-Boundary Conditions.

Unstable Conditions

The Manins (1979) plume penetration model is used for unstable conditions:

$$\begin{aligned} f &= \text{fraction of the plume remaining within the mixing layer} \\ &= 0.08 \left(1 + \frac{1}{P} \right) - P \end{aligned} \quad (4.126)$$

where:

$$P = \frac{F_B}{U_p b_I (Z_i - Z_s)^2} \quad (4.127)$$

$$\begin{aligned} U_p &= \text{wind speed at plume height (m/s)} \\ F_B &= \text{buoyancy flux of the release (m}^4/\text{s}^3) \text{ (Equation 4.103)} \\ b_I &= \text{strength of the inversion (m/s}^2) \\ &= g (\Delta\theta_I)/\theta_A \\ \Delta\theta_I &= \text{change in potential temperature across the depth of the inversion (K)} \\ &= 10 \text{ K (Ley, 1986)} \\ Z_i &= \text{mixed layer height (m)} \\ Z_s &= \text{source height (m)} \\ \theta_A &= \text{potential temperature at plume height (K) (Equation 4.84).} \end{aligned} \quad (4.128)$$

This model is simple as it is based on buoyancy flux rather than plume rise (as is the penetration model for neutral atmospheres). By only considering F_B , it is felt that plume penetration for unstable conditions will err on the conservative side. It is anticipated that plume penetration will be an important factor for ignited release cases where the buoyancy rise will clearly dominate the momentum rise.

The plume rise of the mass remaining in the mixed layer is:

$$Z_{PF,PEN} = Z_i \quad (4.129)$$

where $Z_{PF,PEN}$ = the final plume elevation from the penetration model (m).

When the plume reaches $0.67 Z_{PF,PEN}$, the fraction f is allowed to decrease linearly from 1.0 to the calculated value of f at the final rise elevation $Z_{PF,PEN}$. The value for f is not allowed to be less than f_{MIN} as discussed later in this subsection.

Neutral Conditions

From the final plume rise estimates, it is possible to predict if the jet/plume will interact with the top of the mixed layer. If some of the plume penetrates the mixed layer, then downwind ground-level concentrations of toxic gas will be proportionally reduced. If f represents the fraction of the plume remaining below the mixed layer height Z_i , then OME (1986) suggests:

$$\begin{aligned} f &= 1 & \text{if } Z_i > Z_s + 1.5 \Delta h \\ f &= (Z_i - Z_s)/\Delta h - 0.5 & \text{if } Z_s + 0.5 \Delta h < Z_i < Z_s + 1.5 \Delta h \\ f &= f_{MIN} & \text{if } Z_i < Z_s + 0.5 \Delta h \end{aligned} \quad (4.130)$$

where: Z_i = mixed layer height (m)
 Z_s = height of the "S" plane (or the "C" plane, if there is ignition) (m)

Δh = final plume rise estimate, as in Section 4.3 (m).

Figure 4.7 illustrates the above relationships schematically. The value for f is not allowed to be less than f_{MIN} as discussed later in this subsection. When the plume reaches $0.67 Z_{PF, PEN}$, the fraction f is allowed to decrease linearly from 1.0 to the calculated value of f at the final rise elevation $Z_{PF, PEN}$. If plume penetration is predicted to occur ($f < 1$), then the final elevation of the plume is given as (OME, 1986):

$$Z_{PF, PEN} = \text{MIN} \left[\frac{(Z_i + Z_s)}{2} + \frac{\Delta h}{4}, Z_i \right] \quad (4.131)$$

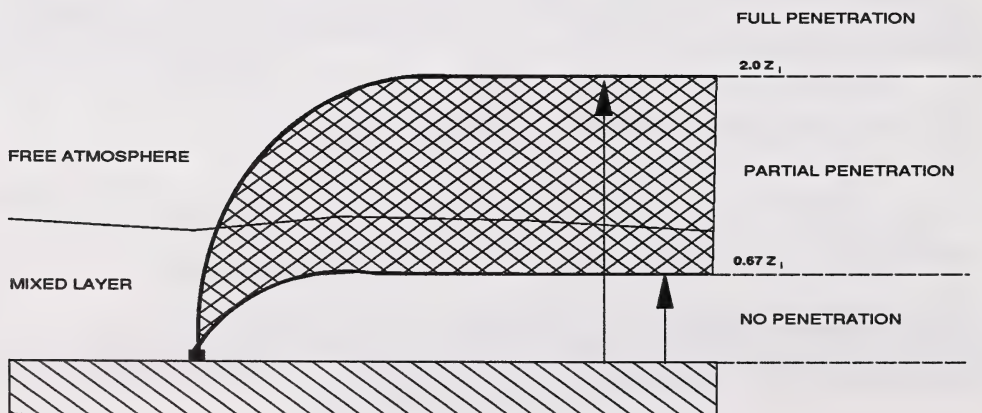


Figure 4.7

Plume Penetration Factor f as a Function of Plume Height and Mixing Height for Neutral Conditions.

Stable Conditions

Under stable conditions, unlimited mixing is assumed to occur and the plume penetration concept is not applicable. The mixing layer height is the elevation at which turbulence is a minimum. If the plume rises beyond the top of the mixed layer height, all of the mass released is allowed to disperse downwards, but with the smaller level of turbulence encountered at the higher elevations. Thus for stable conditions:

$$f = 1.0$$
$$Z_{PF,PEN} = Z_{PF,BRIGGS} \quad (4.132)$$

Minimum Penetration

As a plume rises through the mixing layer, portions of the plume edge are expected to be entrained into the mixing layer due to atmospheric and plume generated turbulence which would preclude complete penetration. That is, f should never equal zero. For this reason a minimum value for f is estimated from:

$$f_{MIN} = f + f_{EDGE}(1 - f) \quad (4.133)$$

where:

- f_{MIN} = Minimum value of f used in dispersion equations.
- f = Predicted values of f .
- f_{EDGE} = Entrainment value to define f_{MIN}
= 0.05

The value of f_{EDGE} is expected to be a function of atmospheric stability and the time the plume spends in the mixing layer. Larger levels of turbulence and longer times in the mixing layer are expected to contribute to producing a larger value of f_{EDGE} . In the absence of observations for f_{EDGE} , a single value of 0.05 is recommended. If f_{EDGE} is set to 1.0 by the user, all of the mass released stays in the mixed layer.

4.5.2 Adjustment of Crosswind Plume Spreads for Averaging Time

The crosswind or horizontal plume spread values used in this work are interpreted to be representative of 30-minute averaging times. Often, concentrations are required for another averaging time, needing a conversion of the horizontal plume spreads from the 30-minute value to the specified value. The formulation used in this work is (e.g., Pasquill and Smith, 1983):

$$\frac{\sigma_{Y2}}{\sigma_{Y1}} = \left(\frac{t_2}{t_1} \right)^{q_T} \quad (4.134)$$

where: σ_{Y1} = horizontal plume spread for averaging time t_1 (m)
 t_1 = averaging time (s)
 σ_{Y2} = horizontal plume spread for averaging time t_2 (m)
 t_2 = averaging time (s)
 q_T = an exponent which depends on atmospheric stability

There is some variation in the literature as to the appropriate values to use for q_T . A value of 0.2 is used in this work, as suggested by Alberta Environment.

Vertical plume spread values do not require an adjustment for averaging time.

4.5.3 Elevated Versus Surface Release Criteria

The criteria for determining whether a plume is classified as an elevated release (as opposed to a surface release) are:

$$Z_{PF,MAX} > 20Z_o + 3 \quad (4.135)$$

or

$$Z_F > 0.565\sigma_{ZF}$$

where: $Z_{PF,MAX}$ = final height of the plume above ground level (m)
 Z_o = surface roughness length (m)
 Z_F = height of plume at X_F (m)
 σ_{ZF} = initial vertical plume spread at X_F assuming elevated release (m).

For a surface roughness of 0.1 m, the final plume height must be greater than 5 m for the release to be modelled as an elevated release. The second criteria is for releases which impinge on or scuff the ground. This criteria prevents higher ground level concentrations being predicted from elevated releases than from surface releases.

4.5.4 Elevated Releases

Elevated plume releases assume the frequently used Gaussian plume model (e.g. Turner, 1970). This model assumes that the distribution of plume material in the vertical and crosswind directions have a Gaussian or normal distribution. The ground level concentration is given by:

$$\chi_i(x, y, z) = \frac{f \dot{m}_p}{2\pi U_p \sigma_{y_i} \sigma_z} \exp\left(-\frac{y^2}{2\sigma_{y_i}^2}\right) g \quad (4.136)$$

where: $\chi_i(x, y, z)$ = concentration of a given plume component (H_2S or SO_2) at position (x, y, z) averaged over t minutes (kg/m^3)

x = downwind distance from the rupture point (m)

y = crosswind distance (m)

z = height above ground level (m)

f = fraction of the plume remaining below the mixed layer height

$\dot{m}_p$ = mass flow of the given plume component (H_2S or SO_2) in the release (kg/s)

U_p = wind speed at plume height (m/s). The wind speed at plume height is used since an average plume element spends most of its time at this height.

σ_{y_i} = effective standard deviation of the plume in the crosswind direction averaged over t minutes (m)

σ_z = effective standard deviation of the plume in the vertical direction (m)

Z_p = height of the plume above ground level (m)

Z_i = mixed layer height (m).

g = function to account for vertical plume spread, depending on stability.

For stable unlimited mixing:

$$g = g_1$$

For unstable or neutral, plume trapping if $\sigma_z \leq 1.6Z_i$:

$$g = g_1 + g_2$$

For $\sigma_z > 1.6Z_i$:

$$g = g_3$$

where:

g_1 = function to account for plume reflections from ground

$$g_1 = \exp\left[\frac{-(z - Z_p)^2}{2\sigma_z^2}\right] + \exp\left[\frac{-(z + Z_p)^2}{2\sigma_z^2}\right]$$

g_2 = function to account for plume reflections from inversion at mixed layer height Z_i if $\sigma_z \leq 1.6Z_i$

$$g_2 = \sum_{n=1}^{10} \left\{ \exp\left[\frac{-(z - Z_p - 2nZ_i)^2}{2\sigma_z^2}\right] + \exp\left[\frac{-(z + Z_p - 2nZ_i)^2}{2\sigma_z^2}\right] + \exp\left[\frac{-(z - Z_p + 2nZ_i)^2}{2\sigma_z^2}\right] + \exp\left[\frac{-(z + Z_p + 2nZ_i)^2}{2\sigma_z^2}\right] \right\}$$

g_3 = function to account for uniform mixing of plume within mixed layer Z_i if $\sigma_z > 1.6Z_i$

$$g_3 = \sqrt{2\pi} \text{ and set } \sigma_z = Z_i$$

The mass flow of the given plume component $\dot{m}_p$ is a fraction of $\dot{m}_{E,S}$ or $\dot{m}_{EFF}$ (Equation 4.118), depending on the composition of the release.

Virtual Source Distances

The virtual source distance X_s accounts for the initial spread of the plume calculated in the integral plume rise module. The relationships which describe the virtual source concept are given in Table 4.6 and are illustrated in Figure 4.8.

To obtain the virtual distance X_v , the mass flow $\dot{m}_p$ from the top hat profile at X_F is equated to the mass flow of a plume in the free atmosphere with Gaussian concentration profiles in the crosswind and vertical directions. By assuming that the centreline concentration of the Gaussian distribution is equal to the average top hat concentration, the following equation can be solved:

$$2\pi U_F \sigma_{Y3}(X_v) \sigma_z(X_v) = \pi R_F^2 V_F \quad (4.137)$$

Table 4.6

Virtual Source Concept for Elevated Plumes.

The virtual source distance is defined by:

$$X_s = x - X_f + X_v \quad (4.138)$$

where:

- X_s = downwind distance from virtual source (m)
- x = downwind distance from release point to where the ambient concentration is to be calculated (m)
- X_f = downwind distance from release point to where the integral plume rise has terminated (m)
- X_v = virtual distance to account for the initial spread of the plume (m).

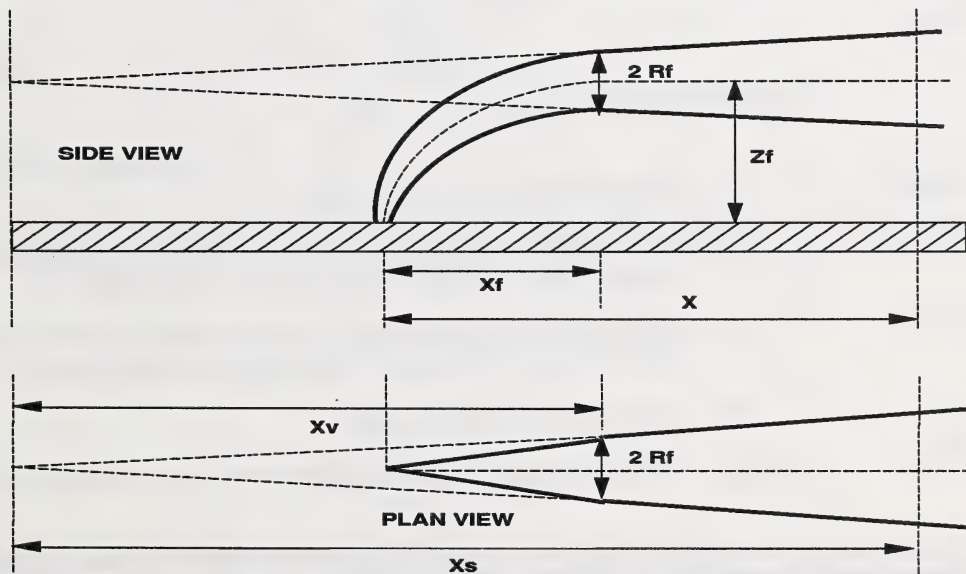


Figure 4.8

Virtual Source Concept for Elevated Plumes.

where: U_F = wind speed at height Z_F (m/s)
 R_F = plume radius when integral plume rise has terminated (m)
 V_F = plume speed at height Z_F (m/s).

A 3-minute averaging time is assumed for crosswind plume spreads. Equations for $\sigma_{Y_{30}}$ (adjusted for averaging time) and for σ_Z are substituted in the above equation and solved for the virtual distance X_v . The equations used to estimate plume standard deviations ($\sigma_{Y_{30}}$ and σ_Z) are stability dependent and are given in the following sections.

Unstable Conditions

For unstable conditions, the Weil and Brower (1984) model is used to estimate plume standard deviations for elevated releases:

$$\sigma_{Y_{30}} = \left[0.0064 + 0.3136 \left(\frac{W^*}{U(0.1Z_i)} \right)^2 \right]^{1/2} X_s f_{CY} \quad (4.139)$$

$$\sigma_Z = \left[0.0036 + 0.3136 \left(\frac{W^*}{U(0.1Z_i)} \right)^2 \right]^{1/2} X_s f_{CZ} \quad (4.140)$$

where: X_s = distance from a virtual source (m),
 f_{CY} = dimensionless correction factor to force the Weil and Brower σ_Y values to equal the Briggs (1974) σ_Y values at large distances,
 f_{CZ} = dimensionless correction factor to force the Weil and Brower σ_Z values to equal the Briggs (1974) σ_Z values at large distances,
 W^* = convective velocity scale (m/s),
 $U(0.1Z_i)$ = wind speed evaluated at 1/10 of the mixed layer height Z_i (m/s).

The correction factors f_{CY} and f_{CZ} are required since the Weil and Brower σ_Y and σ_Z values are only applicable near the source. These factors ensure that the Weil and Brower values converge to the σ_Y and σ_Z values given by Briggs (1974) for large downwind distances. The Briggs values are applicable to open country conditions for downwind distances less than 10 km. The correction factors were empirically determined to be:

$$f_{CY} = \frac{1}{1 + \frac{X_S}{30,000}} \quad (4.141)$$

$$f_{CZ} = \left\{ \left[\left(\frac{U_{REF}}{6W^*} \right)^{0.12} X_S^{(0.04 - 0.011U_{REF}/W^*)} \right]^2 + \left[\frac{300U_{REF}^2}{(13.9W^*)^2 (400 + X_S^{0.75})} \right]^2 \right\}^{1/2} \quad (4.142)$$

Neutral Conditions

For neutral conditions, the Briggs' (1974) model corresponding to open country conditions for downwind distances less than 10 km is used to estimate plume standard deviations for elevated releases:

$$\sigma_{Y30} = \frac{0.08X_S}{(1 + 0.0001X_S)^{1/2}} \quad (4.143)$$

$$\sigma_Z = \frac{0.06X_S}{(1 + 0.0015X_S)^{1/2}} \quad (4.144)$$

Stable Conditions

For stable conditions, the following model is used to estimate plume standard deviations for elevated releases:

$$\sigma'_{Y30} = \frac{\sigma'_{V30}X_S}{U_P} f_Y \quad (4.145)$$

$$\sigma'_Z = \frac{\sigma'_W X_S}{U_P} f_Z \quad (4.146)$$

where:

σ'_{Y30} = passive standard deviation of the plume in the crosswind direction averaged over 30 minutes (m)

σ'_Z = passive standard deviation of the plume in the vertical direction (m)

σ'_{V30} = standard deviation of the crosswind speed fluctuations averaged over 30 minutes (m/s)

σ'_W = standard deviation of the vertical wind speed fluctuations (m/s)

U_p = wind speed at plume height (m/s)

f_y = dimensionless function which relates crosswind velocity fluctuations to crosswind plume spread

f_z = dimensionless function which relates vertical wind velocity fluctuations to vertical plume spread.

Based on Nieuwstadt (1984) and Weil (1985), the standard deviation of the vertical velocity fluctuation can be estimated from:

$$\sigma'_w = 1.3U^* \left(1 - \frac{Z_p}{Z_i}\right)^{3/4} \quad (4.147)$$

where U^* is the surface friction velocity (m/s).

Based on the Hanna (1981) and Pasquill and Smith (1983) interpretations of the 1973 Minnesota Experiment turbulence data (Kaimal *et al*, 1978) and Weil (1985), the standard deviation of the crosswind velocity fluctuation can be estimated from:

$$\sigma'_{v_{30}} = 1.94U^* \left(1 - \frac{Z_p}{Z_i}\right)^{3/4} \quad (4.148)$$

The "3/4" power is an average of the "1" power recommended by Hanna (1981) and the "1/2" power recommended by Pasquill and Smith (1983). The "3/4" value is also consistent with formulation used to estimate σ_w .

The Gaussian plume model assumes that plume spreads are constant with height whereas Equations 4.147 and 4.148 assume that they vary with height. The ratio of (Z_p/Z_i) is set to 1.0 if it is greater than 1.0. For example, the value for σ'_w varies from $1.3 U^*$ at $Z_p = 0$ to zero at $Z_p = Z_i$. Similarly, $\sigma'_{v_{30}}$ varies from $1.94 U^*$ at $Z_p = 0$ to zero at $Z_p = Z_i$. The arithmetic average values of $\sigma'_{v_{30}}$ and σ'_w between height $Z = 0$ and $Z = Z_p$ are used in this model:

$$\begin{aligned}\sigma'_{v_{30}} &= 0.820 U^* \left[1 + \left(1 - \frac{Z_p}{Z_i} \right)^{3/4} \right] \quad \text{if } Z_p < Z_i \\ &= 0.820 U^* \quad \text{if } Z_p \geq Z_i\end{aligned}\tag{4.149}$$

$$\begin{aligned}\sigma'_w &= 0.650 U^* \left[1 + \left(1 - \frac{Z_p}{Z_i} \right)^{3/4} \right] \quad \text{if } Z_p < Z_i \\ &= 0.650 U^* \quad \text{if } Z_p \geq Z_i\end{aligned}\tag{4.150}$$

The above values for $\sigma'_{v_{30}}$ and σ'_w are a modified version of Wilson's (1987) recommendations. The arithmetic average, rather than the time weighted average suggested by Wilson, is used.

The dimensionless functions f_Y and f_Z are taken from Pasquill (1976) and Irwin (1983):

$$f_Y = \frac{1}{1 + \left(\frac{X_s}{2500} \right)^{1/2}} \quad \text{for} \quad X_s \leq 10^4 \text{ m} \tag{4.151}$$

$$f_Y = \frac{33}{X_s^{1/2}} \quad \text{for} \quad X_s > 10^4 \text{ m}$$

$$f_Z = \frac{1}{1 + 0.9 \left(\frac{X_s}{50U_p} \right)^{1/2}} \tag{4.152}$$

The function f_Y has the property of equalling one at $X_s = 0$ m and decreasing to 0.33 at $X_s = 10^4$ m. Similarly f_Z also equals one at $X_s = 0$ m and decreases to 0.10 at $X_s = 10^4$ m (with $U_p = 2$ m/s).

The passive plume standard deviations decrease as the plume travels upward through the mixed layer encountering lower turbulence. The total or effective plume standard deviations are determined from:

$$\sigma_{Y_3} = \left[(\sigma'_{Y_3})^2 + (\sigma'_{Y_{3F}})^2 \right]^{1/2} \quad (4.153)$$

$$\sigma_Z = \left[(\sigma'_Z)^2 + (\sigma'_{Z_F})^2 \right]^{1/2} \quad (4.154)$$

where:

σ'_{Y_3} = passive spread of plume in crosswind direction averaged over 3 minutes with $X_V = 0$ (m)

$\sigma'_{Y_{3F}}$ = initial spread of plume in crosswind direction at X_F averaged over 3 minutes (m)

σ'_Z = passive spread of plume in vertical direction with $X_V = 0$ (m)

σ'_{Z_F} = initial spread of plume in vertical direction at X_F (m).

The passive plume spreads allow for the growth of the plume relative to the initial plume spread at X_F . The virtual distance X_V is set equal to zero for calculations of the passive plume spreads, so the downwind distance is relative to X_F . The initial plume spreads are the values obtained from solving for the virtual source distance. The total crosswind plume spread is adjusted for averaging time as required.

4.5.5 Surface Releases

For near surface plume releases, van Ulden's (1978) model is used to estimate crosswind integrated (CWI) ground level plume concentrations. The distribution of plume material in the crosswind direction is assumed to have a Gaussian or normal distribution. The vertical spread of the plume is assumed to follow the exponential form given by Horst (1979). With these assumptions, the ambient concentration is given by:

$$\chi_i(x, y, z) = \frac{0.73f\dot{m}_p}{\sqrt{2\pi}\bar{U}\sigma_{y_t}\bar{Z}} \exp\left(-\frac{y^2}{2\sigma_{y_t}^2}\right) \exp\left[-\left(\frac{z}{1.52\bar{Z}}\right)^{\frac{3}{2}}\right] g \quad (4.155)$$

where: $\chi_i(x, y, z)$ = concentration of a given plume component (H_2S or SO_2) at position (x, y, z) averaged over t minutes (kg/m^3)

x = downwind distance from the rupture point (m)

y = crosswind distance (m)

z = height above ground level (m)

f = fraction of the plume remaining below the mixed layer
height = 1.0

$\dot{m}_p$ = mass flow of the given plume component (H_2S or SO_2) in the release
(kg/s)

$\bar{U}$ = mean transport wind speed for the plume (m/s)

$\bar{Z}$ = mean height to which plume has dispersed (m)

σ_{y_t} = standard deviation of the plume in the crosswind direction averaged
over t minutes (m).

g = function to account for uniform mixing if $\bar{Z} > Z_i$
stable, unlimited mixing
= 1
neutral and unstable, inversion at Z_i
= $1/0.73$ and $\bar{Z} = Z_i$.

The mass flow of the given plume component $\dot{m}_p$ is a fraction of $\dot{m}_{E,S}$ or $\dot{m}_{EFF}$, depending on the composition of the release. The effective mass flow $\dot{m}_{EFF}$ is a function of the along wind dispersion σ_{x_1} which is, in turn, a function of the vertical dispersion σ_z and plume height Z_p . The following relationships have been used to estimate $\dot{m}_{EFF}$ for surface releases:

$$Z_p = \bar{Z} \quad (4.156)$$

$$\sigma_z = 1.3\bar{Z}$$

Virtual Source Distances

The virtual source distances (X_{SY} and X_{SZ}) account for the initial spread of the plume and the non-zero release height. The relationships which describe the virtual source concept are given in Table 4.7 and are illustrated in Figure 4.7.

To obtain the virtual distances (X_{VY} and X_{VZ}), the mass flow $\dot{m}_p$ from the top hat profile at X_F is equated to the mass flow of a ground based plume with a Gaussian concentration profile in the crosswind direction and an exponential profile in the vertical direction. If the concentration of the ground based profile at $y = 0$ and $Z = \bar{Z}$ is assumed equal to the average top hat concentration, the following equation can be solved:

$$\frac{\sqrt{2\pi}}{0.73} \bar{U} \sigma_{Y_3}(X_{VY}) \bar{Z}(X_{VZ}) \exp\left[\left(\frac{1}{1.52}\right)^{3/2}\right] = \pi R_F^2 V_F \quad (4.156)$$

To solve the above equation, σ_{Y_3} is forced to be equal to the scuffed plume radius divided by $\sqrt{2}$, thus X_{VZ} can be obtained. The virtual distance X_{VY} is then obtained by solving:

$$\sigma_{Y_3}(X_{VY}) = \frac{R_F}{\sqrt{2}\sqrt{f_A}} \quad (4.157)$$

where f_A is the area reduction factor at X_F to account for plume scuffing.

The methods for estimating the plume crosswind standard deviation (σ_{Y_i}), the mean transport wind speed ($\bar{U}$) and the mean plume height ($\bar{Z}$) are stability dependent and are given in the following sections.

Table 4.8

Virtual Source Concept for Surface Plumes.

The virtual source distances are defined by:

$$X_{SY} = x - X_F + X_{VY} \quad (4.158)$$

$$X_{SZ} = x - X_F + X_{VZ} \quad (4.159)$$

where:

- x = downwind distance from release point to where the ambient concentration is to be calculated (m)
- X_F = downwind distance from release point to where the integral plume rise has terminated (m)
- X_{VY} = virtual distance to account for the initial crosswind spread of the plume (m)
- X_{VZ} = virtual distance to account for a non-zero ground release in the estimation of vertical exponential profile (m).

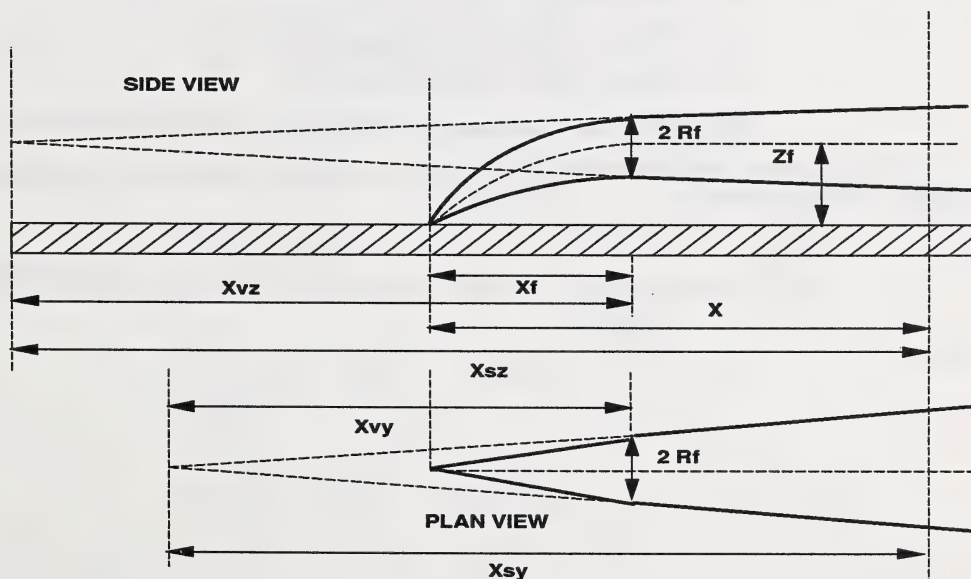


Figure 4.9

Virtual Source Concept for Surface Plumes.

Unstable Conditions

For surface releases under unstable conditions:

$$\sigma_{Y30} = \frac{0.6Z_i X_{SY}^*}{(1 + 0.7X_{SY}^*)^{1/2}} f_Y \quad (4.160)$$

$$\bar{Z} = 0.812Z_i X_{SZ}^{*3/2} \quad \text{if } \bar{Z} < Z_i \quad (4.161)$$

$$= Z_i \quad \text{if } \bar{Z} \geq Z_i$$

$$\bar{U} = U(\bar{Z}) \quad (4.162)$$

where:

X_{SY}^* = non-dimensional distance from a virtual y-source

$$= \frac{X_{SY} W^*}{U_{REF} Z_i}$$

X_{SZ}^* = non-dimensional distance from a virtual z-source

$$= \frac{X_{SZ} W^*}{U_{REF} Z_i}$$

Z_i = height of the mixed layer (m)

W^* = convective velocity scale (m/s)

X_{SY} = distance from a virtual y-source (m)

X_{SZ} = distance from a virtual z-source (m)

$U(\bar{Z})$ = wind speed at mean plume height (m/s)

The dimensionless function which relates crosswind velocity fluctuations to crosswind plume spread is given by:

$$f_Y = \frac{1}{1 + \frac{x_{SY}}{30000}} \quad (4.163)$$

Neutral Conditions

For surface releases under neutral conditions:

$$\sigma_{Y_{30}} = \frac{\sigma_{V_{30}} X_{SY}}{U_{REF}} f_Y \quad (4.164)$$

The mean plume height $\bar{Z}$ is given by the solution of:

$$X_{SZ} = \frac{0.74\bar{Z}}{k^2} \ln\left(\frac{0.6\bar{Z}}{Z_o}\right) \quad (4.165)$$

The maximum value of $\bar{Z}$ is Z_i . The mean wind speed $\bar{U}$ is given by:

$$\bar{U} = \frac{U^*}{k} \ln\left(\frac{0.6\bar{Z}}{Z_o}\right) \quad (4.166)$$

where: U^* = surface friction velocity (m/s)
 k = von Karman constant (~ 0.4)
 Z_o = surface roughness length (m).

The standard deviation of the crosswind speed fluctuations is given by:

$$\sigma_{V_{30}} = 1.3U^* \quad (4.167)$$

The dimensionless function f_Y is based on Pasquill (1976) and Irwin (1979):

$$f_Y = \frac{1}{1 + \left(\frac{X_{SY}}{2500}\right)^{1/2}} \quad \text{for} \quad X_{SY} \leq 10^4 \text{ m} \quad (4.168)$$
$$f_Y = \frac{33}{X_{SY}^{1/2}} \quad \text{for} \quad X_{SY} > 10^4 \text{ m}$$

Stable Conditions

For stable conditions, the following model is used to estimate plume standard deviation for surface releases:

$$\sigma'_{Y_{30}} = \frac{\sigma'_{V_{30}} X_{SY}}{U_{REF}} f_Y \quad (4.169)$$

The mean plume height is obtained by solving the implicit equation:

$$X_{SZ} = \frac{0.74\bar{Z}}{k^2} \left\{ \ln \left(\frac{0.6\bar{Z}}{Z_o} \right) + 4.9 \frac{\bar{Z}}{L} \right\} \left[1 + \frac{4.9\bar{Z}}{L} \right] + \frac{1.2\bar{Z}}{L} \quad (4.170)$$

The mean wind speed is given by:

$$\bar{U} = \frac{U^*}{k} \left[\ln \left(\frac{0.6\bar{Z}}{Z_o} \right) + 4.7 \frac{\bar{Z}}{L} \right] \quad (4.171)$$

The standard deviation of the crosswind velocity fluctuation is estimated from the same relationship used for elevated plumes in stable atmospheres:

$$\begin{aligned} \sigma'_{V_{30}} &= 0.820 U^* \left[1 + \left(1 - \frac{\bar{Z}}{Z_i} \right)^{3/4} \right] \quad \text{if } \bar{Z} < Z_i \\ &= 0.820 U^* \quad \text{if } \bar{Z} \geq Z_i \end{aligned} \quad (4.172)$$

The dimensionless function f_Y is based on Pasquill (1976) and Irwin (1979):

$$f_Y = \frac{1}{1 + \left(\frac{X_{SY}}{2500} \right)^{1/2}} \quad \text{for} \quad X_{SY} \leq 10^4 \text{ m} \quad (4.173)$$

$$f_Y = \frac{33}{X_{SY}^{1/2}} \quad \text{for} \quad X_{SY} > 10^4 \text{ m} \quad (4.174)$$

The total or effective crosswind plume standard deviations are determined from:

$$\sigma_{Y_3} = \left[(\sigma'_{Y_3})^2 + (\sigma'_{Y_{3F}})^2 \right]^{1/2} \quad (4.175)$$

Note that X_{VY} is set equal to zero for calculation of σ'_{Y_3} . The total crosswind plume spread is adjusted for averaging time.

4.5.6 Low Wind Speed Stable Conditions

Due to the importance of low wind speed, stable conditions in modelling the dispersion of uncontrolled sour gas releases, some further discussion on the subject is warranted.

Under these conditions, plume meandering can increase the horizontal plume spread values (σ_{y_r}). The longer the averaging period, the larger the value of σ_{y_r} becomes. For the estimation of three-minute average concentrations, the meandering effect is expected to be minimal. The estimation of hourly average concentrations using models which ignore plume meander has led to overpredictions ranging from a factor of 10 for flat terrain to a factor of 100 for rolling forested terrain (Draxler, 1984; Van der Hoven, 1976).

The equations for σ_{y_r} do not account for plume meander. Therefore, caution should be exercised in the interpretation of the low wind speed (less than 3 m/s) plume spreads in stable atmospheres, especially for averaging periods larger than 3 minutes.

4.5.7 Site Specific Turbulence Data

Provisions have been made to allow the user to input site specific measurements of the standard deviation of windspeed fluctuations ($\sigma_{v_{30}}$ and σ_w). The site specific crosswind speed standard deviations must be for a 30-minute averaging time. In addition, the user can input the friction velocity U^* , the convective velocity W^* , the temperature gradient dT_A / dZ and the Monin-Obukhov length L . The reference height Z_{REF} corresponds to the elevation where the windspeed is measured.

4.6 Fluctuating Load and Probit Module

This section discusses the probit analysis (Sections 4.6.1 to 4.6.4) and the fluctuating load (Sections 4.6.5 and 4.6.6) module which has been incorporated in the main modelling system of GASCON2. In addition, a discussion on risk-related calculations which are incorporated in GASCON2 follows (Sections 4.6.7 and 4.6.8).

4.6.1 Probit Analysis

There are a number of data analysis methods which can be used to estimate the probability of lethality due to toxic gas exposure. Foremost among these are probit analysis, logit analysis, the Weibull model, and one-hit and multi-hit models (Morris *et al.* 1984). To our knowledge, the only such method which has been reported in the literature to assess risk associated with episodic chemical releases is probit analysis (Covo (Rijnmond) 1982; Lees, 1980; Withers and Lees, 1985; Poblete and Lees, 1984; Health and Safety Executive, 1978); Eisenberg *et al.* (1975); Ride (1984); Griffiths and Megson (1984); Ten Berge *et al.* (1986); G. Purdy, private communication (1987). These authors indicate the general acceptance by the European technological community of the appropriateness of applying probit analysis to the estimation of hazard and risk resulting from acute exposure to chemical vapours. For this reason, probit analysis is employed in GASCON2 to estimate the lethality of H₂S gas to humans.

Probit analysis estimates the frequency of fatalities in a population of biological organisms (e.g. human beings, cats, dogs, etc.) due to an exposure to a potentially harmful substance (e.g. H₂S, drugs, radiation, etc.). The use of probit equations in hazard and risk assessment is a relatively new development (see references above), although probit analysis dates back to the work of Bliss (1934), and experiments on dose response behavior, which is the basis of probit analysis, date back to the late nineteenth century.

As pointed out by Morris *et al.* (1984) and Krewski and Brown (1981), several dose-response analytical models, such as those mentioned previously, have been evaluated with respect to low-dose extrapolation validity for chronic (as compared with acute) chemical exposures. In this dose-response regime, and particularly for carcinogens or genotoxic chemicals, other models are considered to be more appropriate than the probit model. That is, the probit model may underestimate response at low dosage, if the effect being estimated is believed to require a linear extrapolation model, rather than the exponential form of the probit (log-normal) model. In the case of H₂S, however, there is no evidence of increased mortality to indicate the need for such a treatment at low dosage (Beauchamp *et al.* 1984; NRC, 1979; NRCC, 1981).

The probit model admits some contribution to H₂S-caused mortality at low dosage, including dosage that may be below a detoxification threshold. It is suggested, therefore, that the probit model is a reasonable analytical approach, since it predicts responses intermediate between the linear extrapolation and threshold models (see Harris *et al.* 1984). The applicability of the probit model at the high dosage end (high percentage mortality) is not a critical question, since its validity up to at least the 90th percentile seems well-supported in the literature (see Engeman *et al.* 1986), and above that percentile, over-or under-estimates of mortality will have no practical effect on the risk estimation result.

In addition to the literature on analysis of technological hazards cited above, there is also strong support for the use of probit analysis of acute exposure dose - response data in the toxicological literature. A few selected examples of the latter are Engeman *et al.* (1986), Morgan *et al.* (1982), Papermaster and Pinsus (1974) and Stephan (1977), in addition to the more general position put forward by Finney (1971a). The assumption of a log-normal population response to acute chemical exposures is thus well-supported in the literature.

Toxic Load - Generalized Dose

Since the probit function relates population response to chemical dose, it is important to understand the toxicological parameters that are used to represent dose. The following provides a brief background to this subject as preface to a more detailed mathematical treatment of the probit analysis.

Experimental studies conducted by Lehmann during the period 1887 - 1899 in Germany focussed on determining the effect on animals of exposure time to various toxic gases inhaled at a constant concentration. Later, during the first World War, Haber conducted experiments on animals to determine the toxic effect of chlorine, phosgene and mustard gas inhalation and quantified the roles of toxic gas concentration and exposure time which has since been called Haber's Rule:

$$L = \chi_{t_E} \cdot t_E \quad (4.176)$$

where: L = toxic load (ppm•min)
 χ_{t_E} = toxic gas concentration averaged over t_E minutes (ppm)
 t_E = exposure time (min).

This rule states that the toxic load (L), or dose, which is an indicator of toxic effect, is the product of the concentration (χ_{t_E}) and the exposure time (t_E) of that concentration. Haber's Rule shows that concentration level alone is not sufficient to determine the lethal effect on biological organisms; exposure time also has an effect. L as defined in Equation 4.176 can be related to the total amount of toxic gas inhaled by the test animal according to its rate of respiration. This quantity, in turn, can be related to the dose administered in typical toxicological feeding studies (e.g., for drug testing on food additive testing). Thus, although the parameters are related, it is useful to differentiate between ingested quantity (dose - a measured quantity of chemical administered all at once or in discrete amounts) and inhaled quantity (toxic load - a surrogate for amount taken up as a result of prolonged breathing).

Since the pioneering work of Haber, extensive work by toxicologists has tended to support a somewhat more general presentation of the toxic load:

$$L = \chi_{t_E}^n \cdot t_E \quad (4.177)$$

where the variables take on the same meanings as for Equation 4.176, but the units of the toxic load (L) are ppm ^{n} •min, and n is an index, usually greater than 1.0. This modification to Haber's Rule states that a better indicator of lethality is the concentration (χ_{t_E}) raised to the power " n " times the exposure time (t_E). Since n is usually greater than 1.0, Equation 4.177 suggests that concentration is more important than exposure time in arriving at a toxic

load. For example, if $n = 2$, then a 1 minute exposure to toxic gas at 2000 ppm produces the same toxic load as a 3 minute exposure to 1150 ppm, and hence both have the same potential for lethality.

The evidence for the validity of the representation in Equation 4.177 comes from the analysis of experimental toxicological data, as described by Finney (1971a) and supported by such recent analyses of acute chemical hazards as Withers and Lees (1985), Poblete and Lees (1984), ten Berge *et al.* (1986) and Eisenberg *et al.* (1975). Qualitatively, this representation is based on the observation that the mortality experience of an exposed population in toxicological experiments is often observed to depend more strongly on the concentration than on the time of exposure. This dominance of concentration (χ) over time (t_E) can be determined from statistical analysis of experimental data which is independent of the specific response model that is used (e.g., probit, etc.). The probit function is a means of incorporating the toxic load representation, whether in the simple form of Haber's Rules (Equation 4.176) or in the general form of Equation 4.177, into an analytical expression for response.

The power n is strongly dependent on the toxic gas under consideration. Table 4.8 gives typical values of n for five toxic gases. The value of n alone is **not** a valid measure of the relative toxicity of the gases cited; this will become apparent in subsequent discussions. The value of n may also vary somewhat according the animal species on which the lethality of the toxic gas was examined, since not all species of animals display the same resistance to toxic gas.

Table 4.8

Values of n in $L = \chi^n \cdot t_E$ for various toxic gases.

Toxic Gas	n	Reference
Hydrogen Sulphide (H_2S)	2.50	Rijnmond (1982)
Sulphur Dioxide (SO_2)	2.20	Withers and Lees (1985)
Chlorine (Cl_2)	2.75	Lees (1980)
Ammonia (NH_3)	2.75	Lees (1980)
Carbon Monoxide (CO)	2.00	Withers and Lees (1985)

It is important to be specific about what is meant by "lethality" when discussing probit analysis. Sometimes distinctions are made between "acute" (short term) and "delayed" (long term) deaths due to toxic gas inhalation. For the GASCON2 model, which is primarily concerned with lethality due to H_2S exposure, there are insufficient data in the open literature to discriminate between acute and delayed deaths due to H_2S exposure. Hence, for the GASCON2 model, one can only define "lethality of H_2S " as "deaths directly caused by exposure to H_2S gas," whether acute or delayed.

Probability that Toxic Load is Lethal

A probit analysis of mortality data on subjects exposed to toxic gas results in a probit curve as shown in Figure 4.10. The vertical axis of the graph in the figure is the fraction of the population killed by exposure to the toxic gas. This is equivalent to the probability of lethality for every member of the population. The quantity L_{50} shown on the graph is the toxic load which causes 50% mortality in the population. The L_{10} and L_{90} toxic loads represent

10% and 90% mortality, respectively. Also shown on the graph are the regions of the probit curve representative of the sensitive, average and resistant members of the population. The equation for the probit curve shown in Figure 4.10 is:

$$P(L) = \frac{1}{2} \left[1 + \operatorname{erf} \left(\frac{k_2 \ln(L) + k_1 - 5}{\sqrt{2}} \right) \right] \quad (4.178)$$

where:

$P(L)$ = probability that the toxic load L is lethal
 k_1, k_2 = parameters derived from experimental data
 erf = mathematical error function.

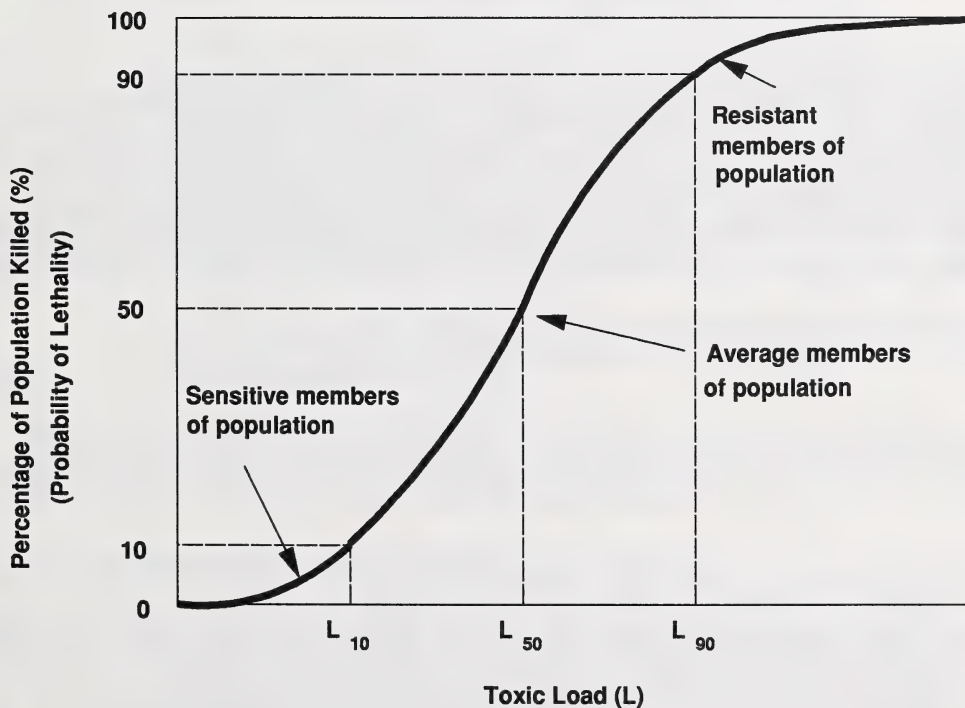


Figure 4.10

An Example of a Probit Curve.

The probit function Y is defined as:

$$Y = k_2 \ln(L) + k_1 \quad (4.179)$$

The logarithmic term arises from the fact that in typical populations, there are some members who can tolerate a high toxic load and others who succumb to a low toxic load. This tends to skew the distribution of frequency of mortality towards the high toxic load end (log-normal distribution).

Equation 4.178 is derived from the defining relationship for $P(L)$ which is found in the literature (Lees 1980; Finney 1971a), namely:

$$P(L) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{Y-5} \exp\left(\frac{-u^2}{2}\right) du \quad (4.180)$$

The probit parameters k_1 , k_2 and n completely determine the probit curve defined by Equation 4.178. These parameters are determined by a maximum likelihood statistical estimation procedure (Finney, 1971a) which minimizes the error between Equation 4.178 and the experimental data of mortality in animals. These probit parameters are required inputs to the GASCON2 model. A discussion of the various H_2S probit parameters considered in this work is given in Section 4.6.2. The relationships between k_1 and k_2 and the experimental data values L_{50} and σ_L (the standard deviation of toxic load for frequency of mortality) are:

$$k_1 = 5 - \frac{\ln(L_{50})}{\sigma_L} \quad (4.181)$$

$$k_2 = \frac{1}{\sigma_L} \quad (4.182)$$

The parameters k_1 , k_2 and n are normally determined for a given set of experimental toxicological data for a controlled group of test animals. The various percentiles (L_{10} , L_{50} , L_{90}) of the response versus toxic load curve may then be read directly. These percentiles would then represent the response of the specific test animal group, interpreted to represent a population. Since there is both quantitative and perceptual difficulty in toxicology to extrapolate animal test results to humans, this approach was not relied on in this study. In the case of H_2S toxicity, there are few data pertaining to human mortality resulting from inhalation of H_2S . Although some toxicologists have expressed the opinion that, for H_2S , the response of the several animal species tested in toxicological studies is similar to that of humans (NRC, 1979), the approach taken to determine the dose-response relationship for this study was to select the parameters by comparison of all available animal data and the few human data, rather than to rely on a single data set. This approach is described in Section 4.6.2.

Discussion

Probit analysis is well-suited to the risk assessment framework employed by GASCON2 for assessing uncontrolled sour gas releases. As has been established by experiment, exposure time to toxic gases is an important consideration in estimating the probability of lethality. Furthermore, some uncontrolled sour gas releases, such as those from pipeline ruptures, may typically last only a few minutes, so that downwind concentrations of H₂S alone are not sufficient to estimate risk; high concentration must be tempered by the relatively short durations (exposure times) over which they occur.

To summarize, the advantages of the probit analysis approach are:

- *Consistency with experimental observations.* Toxic loads defined by Equation 4.177, and the mortality fraction defined by Equation 4.178 predict the mortality response in animals very well (ten Berge, 1986).
- *The ability to account for variable exposure time.* For uncontrolled sour gas releases, downwind concentrations of H₂S can persist for varying lengths of time depending on whether the release is transient (time varying release rate) or steady (constant release rate). Furthermore, even for steady releases, concentration fluctuations due to atmospheric turbulence (see Section 4.6.5) can produce large concentration peaks for small time durations. This indicates that concentration levels alone are not sufficient to quantify the risk to human life posed by uncontrolled releases of sour gas.
- *Simplicity.* The whole range of parameters concerning inhalation toxicity of gases, including concentrations and exposure times, is described by a single equation (Equation 4.178).

Because of the above advantages, the probit analysis approach was incorporated into the GASCON2 modelling system to allow the probability of fatality to be calculated by taking into account the variability of response of the exposed group.

Some limitations of the probit method should also be mentioned:

- *Low dose extrapolation.* As mentioned above, some toxicologists question the validity of the probit model at very low toxic loads, especially in chronic (i.e., extended low-level) exposures, of chemicals whose mode of action does not produce immediate mortality).
- *Extrapolation from animals to human.* Probit analysis suffers the same limitations as any other toxicological model in relating dose-response in one species or strain to that another species or strain, whose physiology and biochemistry may be significantly different.
- *Extrapolation outside experimental data limits.* The principal application of probit analysis is the determination of L₅₀, the toxic load which kills 50% of the test population. Toxicologists have expressed reservations about using the model beyond the L₁₀ and L₉₀ points, the usual limits of accurate experimental data depending upon the application.

- *Sensitivity of results to values of parameters.* The predicted mortality (or risk of mortality) based on a probit function may depend strongly on the specific values of the probit parameters determined or selected for use.

While the potential importance of each of these limitations must be recognized, each has been addressed in this report such that the level of confidence in the approach used here is reasonably strong. Specifically:

- The low dose extrapolation issue has been discussed in section 4.6.1. It was pointed out that the probit model very likely over-estimates the response at low toxic loads, since there is no documented evidence of lethal effects at concentrations less than 100 ppm, regardless of exposure time, which implies that there is a threshold for lethal effects.
- Extrapolation from animals to man has been avoided by selecting the probit parameters based on all available data for various animal species and man, as well as on qualitative observations from the medical case study literature. This approach is described in detail in the next section.
- Since an isolated toxicological experiment was not relied on as the basis for the probit parameters, rather a more extensive body of data and information was used, the issue of extrapolation outside the limits of validity of toxicological data has been alleviated. Weaknesses in data quality are also alleviated by the approach taken. This point is also discussed more fully in the next section.

4.6.2 Probit Parameter Selection

Before the probit approach can be used, it is necessary to select probit parameters which realistically but conservatively, represent human response to acute H₂S exposures. In this section, the H₂S probit parameters which are used in GASCON2 are specified, and the rationale for using these parameters is presented.

The selection of the probit parameters relied on the precedents of the Rijnmond risk analysis (COVO Steering Committee, Rijnmond Public Authority, 1982) and such studies as Withers and Lees (1985), ten Berge *et al.* (1986) and Eisenberg *et al.* (1975) in selecting the probit model as the appropriate relationship among concentration, time and response for lethality of exposure to H₂S. A detailed review of the primary toxicology literature was not carried out, nor was any new analysis of toxicological data performed. Data used were taken from the primary (peer reviewed) literature, from the critical review literature (e.g. Beauchamp *et al.* 1984) and from often cited secondary sources, principally Canadian and U.S. federal government reports.

Several different published data sets and probit equations for a variety of animal species were compared graphically with the relatively few existing data on actual human response to acute H₂S dosages. For these latter human response data, the concentration, time and fractional population response are reasonably well known. These data, along with the literature probit equations and adjusted literature equation are shown in Figure 4.11. The probit curves in Figure 4.11 are plots of probability of lethality for a 3-minute exposure versus concentration in ppm. The probit parameters for each of the five probit curves are summarized in Table 4.09.

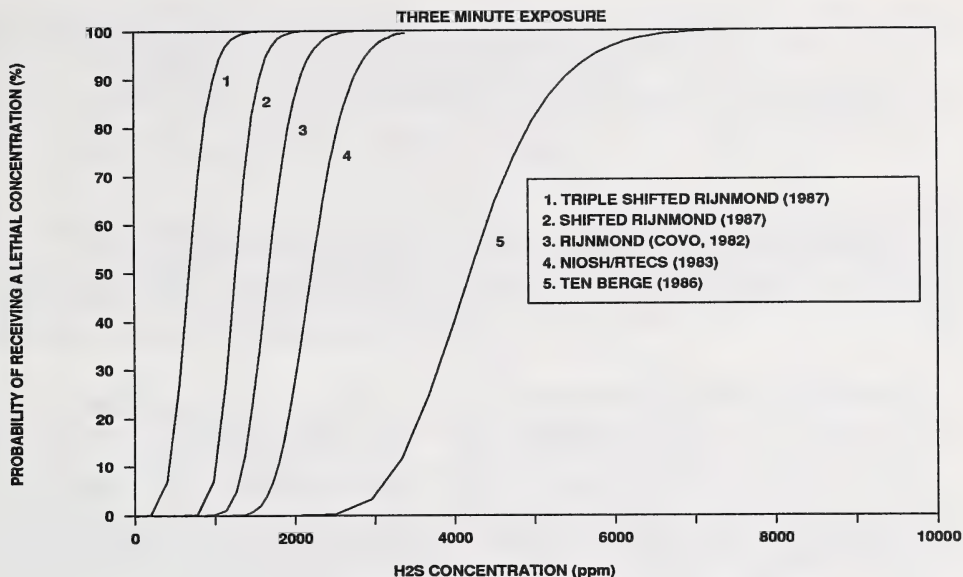


Figure 4.11

Probability of Lethality for a Three-Minute Exposure to H₂S Concentrations for Selected Probit Equations from the Literature.

Table 4.09

H₂S Probit Parameters.

Source	k_1	k_2	n
Triple Shifted Rijnmond	-36.20	2.366	2.5
Shifted Rijnmond	-39.80	2.366	2.5
Rijnmond (COVO, 1982)	-41.48	2.366	2.5
NIOSH/RTECS (1983)	-43.93	2.380	2.5
ten Berge (1986)	-40.90	2.360	2.2

Figure 4.12 shows a graph of known human and animal mortality statistics for H₂S. The graph shows toxic load (L) versus the probit function (Y) from Equation 4.179. The index " n " used in the calculation of toxic load was taken to be $n = 2.5$. Also shown in Figure 4.12 are the three probit functions considered in this work for which $n = 2.5$ (see Table 4.10). Plots of the of probit function (Y) versus toxic load (L) appear as straight lines. The closer a line is to the horizontal axis on the graph, the more conservative the probit function is, that is, the lower the toxic load which can produce a fatal response. The relationship between probit (Y) and probability of lethality ($P(L)$), given by Equations 4.177 and 4.178 is also displayed in the figure.

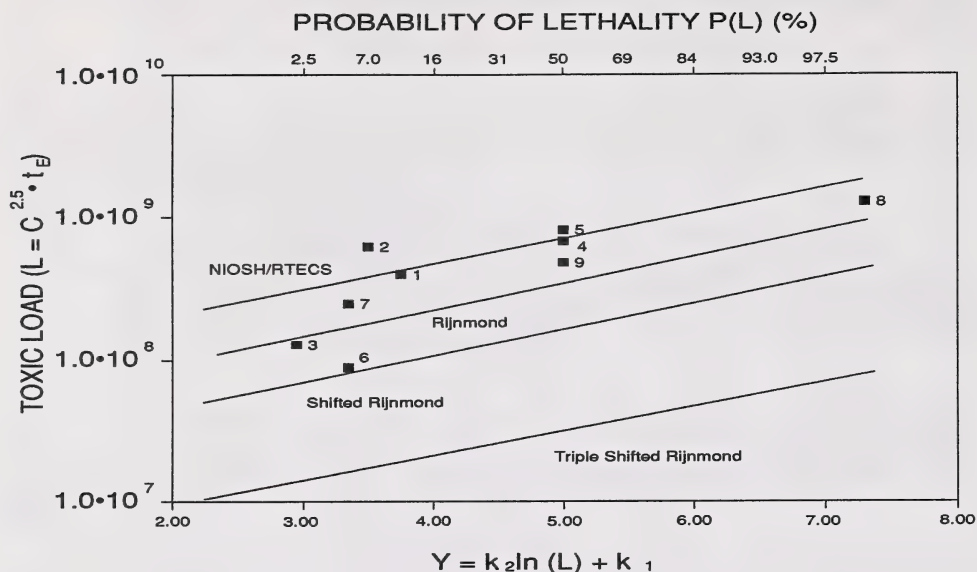


Figure 4.12

Probability of Lethality for a Three-Minute Exposure to H_2S Concentrations for Selected Probit Parameters.

Table 4.10

Key to Symbols in Figure 4.12.

Symbol	Reference	Animal	Toxic Load	Comment
1	NIOSH, 1977	Humans	L_{10}	2800 ppm/1 min (1/10 died)
2	NRC, 1985	Humans	L_7	1000 to 2000 ppm/20 min (22/320 died)
3	Atwell <i>et al.</i> 1979	Humans	L_2	700 ppm/10 min (2/89 died)
4	RTECS, 1983.	Mice	L_{50}	673 ppm/1h
5	Atwell <i>et al.</i> 1979	Rats	L_{50}	713 ppm/1h
6	RTECS, 1983.	Mammals	L_{10}	(taken as L_5) 800 ppm/5 min
7	RTECS, 1983.	Humans	L_{10}	(taken as L_5) 600 ppm/30 min
8	Haggard, 1925 (citing Lehmann, 1892).	Dogs	L_{99}	1500 ppm/15 min
9	Clanachan, 1979.	Mice	L_{50}	Average of $\chi^{2.5}_{t_{95}} = 5.1 \cdot 10^8$. Data from Clanachan and NRCC, 1981 (Table III-4).

The Rijnmond (COVO Steering Committee, 1981) and the ten Berge *et al.* (1981) probit equations for H₂S toxicity were the only two equations found in the literature referring to lethality. A third probit function was generated from points 4 and 1 in Figure 4.12 which are the L_{50} (mice) and L_{10} (humans) from NIOSH data, assuming $n=2.5$ as in the two references cited above. The latter was suggested unofficially by representatives of the Dutch Ministry of the Environment in a private communication.

In a private communication with the Dutch MOE, probit parameters were obtained which had been re-calculated from the same data set used by ten Berge. In our computation of the probability of lethality versus distance from the source of release, the latter proved to be less conservative than the Shifted Rijnmond equation and so was not further considered, particularly because of the lack of documentation.

A fourth probit function was created by adjusting the Rijnmond (COVO, 1982) function k_1 parameter by +1.8 units, such that it would fall below point 6 in Figure 4.12. This has been labelled the "Shifted Rijnmond" function. The intent of this adjustment is to produce a probit equation that is more conservative than the literature values, that is, does not underestimate response indicated by all the available data. Such an adjustment is consistent with the approach taken by Withers and Lees (1985) with respect to chlorine. These authors determined different probit equations for fatality in response to acute exposure to chlorine gas for normal ("regular") and vulnerable human populations. The probit for the vulnerable population was determined to require an adjustment of k_1 only, leaving k_2 and n fixed. They adjusted k_1 by +1.7 units for chlorine.

Although the approach taken by Withers and Lees seems reasonable, it is not based on a detailed analysis of biological models. It assumes that the basic mechanism of action by H₂S is the same for the resistant, average and sensitive sub-populations, as reflected in the consistency of the k_2 and parameters which determines the slope of the curve. This assumption is consistent with what is known about H₂S toxicology (NRCC, 1981; WHO, 1981). The adjustment of the parameter k_1 can be related to a sub-population which is more sensitive than the total population. The effect of the adjustment is to create a sub-population characterized by an L_{50} which is approximately equivalent to the L_{10} associated with the total population (represented by the unshifted Rijnmond equation). This means that the lethal load that would be fatal to 10 percent of the pre-adjusted total population would be fatal to 50 percent of a more sensitive sub-population group which is characterized by shifted Rijnmond function.

A further adjustment to the Rijnmond function is thus advisable. The adjustment of the parameter k_1 to bring the predicted lethality into agreement with the literature on human experience produces the values shown as Triple Shifted Rijnmond in Table 4.10. Figure 4.11 displays the fatal concentrations of H₂S derived from the Triple Shifted Rijnmond equation for selected exposure times. The effect of the additional shift is to produce an L_{50} equivalent to L_1 of the Shifted Rijnmond equation.

Figure 4.13 shows the Triple Shifted Rijnmond probit curve plotted against H₂S concentration in ppm for 1/2, 1, 3, 30 and 60-minute exposure times. The appropriateness of the Triple Shifted Rijnmond function was tested by back-calculating the lethal concentrations for various exposure times and levels of lethality (L_1 , L_{10} , L_{50} , L_{90} and L_{99}). These values are shown in Table 4.12 for 1/2, 1, 3, 30, and 60-minute exposure times.

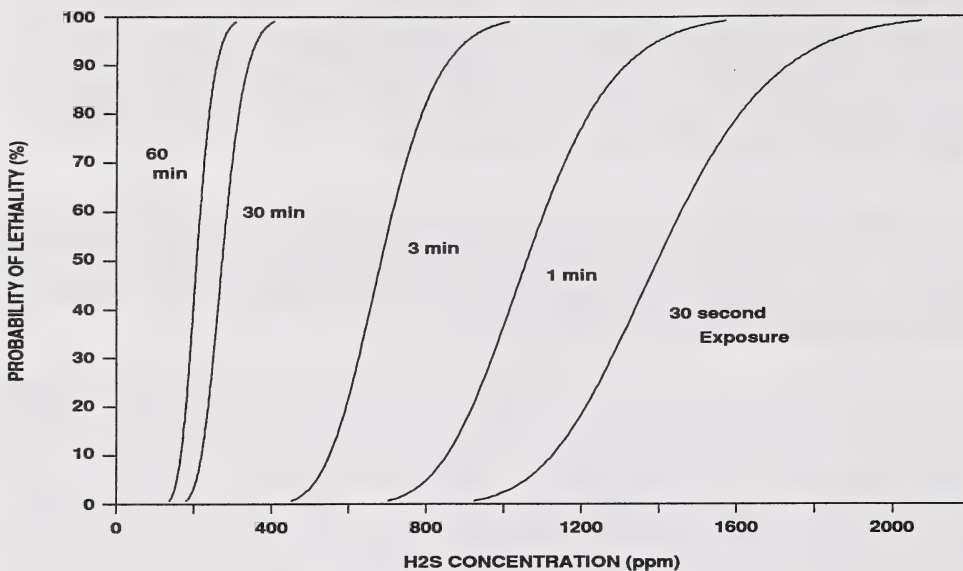


Figure 4.13

Probability of Lethality Based on the Triple Shifted Rijnmond Probit Equation for Selected Exposure Times to H₂S Concentrations.

Table 4.11

Fatal H₂S Concentrations (ppm) Derived from Triple Shifted Rijnmond Probit Function for Selected Exposure Times.

L_x Toxic Load for X% mortality	Exposure Time (min)				
	0.5	1	3	30	60
L_1	945	715	460	185	140
L_{10}	1130	850	550	220	165
L_{50}	1400	1060	680	270	205
L_{90}	1735	1315	845	335	255
L_{99}	2070	1570	1010	400	305

These dose-response data were compared with available literature data, as summarized in NRCC (1981), WHO (1981) and Atwell *et al.* (1979). Table 4.12 shows the concentration levels and exposure times associated with death, based on the judgement of the panel which authored the NRCC (1981) report. Greenhill (1978), in his earlier review of the literature, classified H₂S concentrations according to the following:

- More than 2 000 ppm: Immediate death,
- 1 000 to 2 000 ppm: Death within 30 minutes,
- 700 to 1 000 ppm: Death within 1 hour, and
- 500 to 700 ppm: Death within 4 to 8 hours.

The fatal concentrations predicted by the Triple Shifted Rijnmond function for the exposure times shown in Table 4.11 are comparable with the literature review results presented above and in Table 4.12. The data in Table 4.11 (and the curves in Figure 4.13), however, are less conservative than what has been intuitively assumed and used by the sour gas industry where instantaneous concentrations ranging from 500 to 1000 ppm have been assumed to be lethal (e.g. Angle, 1982; Kropola, 1982; Occupational Health and Safety, 1985).

Table 4.12

H₂S Concentration Range and Exposure Times Causing Death (NRCC, 1981).

H ₂ S Concentration (ppm)	Exposure Time
More than 2 000	seconds to 2 minutes
700 to 1 500	seconds to 15 minutes
500 to 600	2 to 60 minutes
250 to 450	1 to 8 hours
100 to 200	8 to 48 hours

Monserco (1981) carried out a risk analysis associated with episodic exposure to H₂S for the Atomic Energy Control Board. Monserco developed a step function relationship between toxicity and length of exposure based on their reading of the literature. The Monserco criteria for lethality included both death and unconsciousness, and the toxic level for longer-term exposure (10 to 60 min) was based on a study of occupational exposure to H₂S in the shale oil industry, in which no fatalities were reported (Ahlborg, 1951). The Monserco study also used simple dose ($\chi \cdot t_E$) rather than toxic load ($\chi^n \cdot t_E$) and did not use an analytical function (such as probits) to compute dose-response.

Other qualitative summaries of dose-response for H₂S, such as CCOHS (1985) and Canada Safety Council (1980) confirm that the Shifted Rijnmond equation, although conservative with respect to the available animal toxicological and human exposure data (Figure 4.11) is not consistent with other data, including case studies, on which the various literature descriptions of human experience are based.

Population Vulnerability

The most thorough treatment of population vulnerability (or sensitivity) in hazard analysis appears in Withers and Lees (1985). Two important factors are assessed in their work: population vulnerability respecting physiological sensitivity and more severe exposure due to an increased level of physical activity. The latter could be expected in a crisis situation where a community experiences an acute exposure to a toxic gas.

Their adjustment of the response function for population sensitivity is based on the minimum concentration (or load) at which a fatality has actually been observed. The dose-response function (expressed as a probit function based on toxic load) for the vulnerable population is obtained by shifting the function for the "regular" population (which includes an estimated 25% vulnerable individuals) and keeping the same slope (i.e., k_1 is increased while k_2 and n parameters constant). That is, the regular dose-response function is translated to accommodate the most sensitive documented response.

The level of physical activity during a crisis would likely be higher than under the conditions of most of the laboratory toxicological tests. Withers and Lees accounted for this by assuming an inhalation rate of twice the base (resting) level during the exposure period. This adjustment is accomplished by reducing the effective concentrations used in the data analysis by a factor of two. As Withers and Lees point out, a larger factor might be justifiable under certain conditions or for certain groups of people.

The Shifted Rijnmond probit function has been taken to characterize the normal population. The Triple Shifted Rijnmond function, which was used for risk calculation in this report, accounts for the lowest reported lethal load. No specific adjustment was made for level of physical activity, but application of the Triple Shifted function to the entire exposed population (rather than weighting by the proportion of regular and vulnerable individuals, as Withers and Lees did) is intended to achieve a similar level of conservativeness as the Withers and Lees approach.

Sub-Lethal Effects of H₂S and SO₂ Toxicity

In this study, the probit method is applied to lethality of H₂S exposure only. Because of the variety of dose-response relationships for non-lethal effects of exposure to H₂S, and because of the human body's ability to detoxify H₂S after such exposures, the probit model may not be appropriate to apply to sub-lethal effects of exposure to H₂S. A model (or models) incorporating pharmacokinetic parameters of detoxification would be required (Ramsey and Gehring, 1981). It is not known whether there are sufficient data to construct such a model for the general population. Thus, quantitative risk calculations were not made for sub-lethal effects.

While data pertaining to lethal effects of exposure to SO₂ exist, they are not germane to this study because the results of the concentration analysis indicated that the worst-case SO₂ concentrations resulting from ignited sour gas releases were clearly sub-lethal. The sub-lethal effects of SO₂ are not addressed in this study for the same reasons given above respecting H₂S.

Discussion

The use of the probit model to estimate the lethal consequences of exposure to hydrogen sulphide has not been superseded by any other more appropriate analytical approach. The probit approach was presented as the simplest way to incorporate toxicological data into the computational scheme of GASCON2, and its use was supported by reference to growing acceptance by the international risk analysis community. Probit analysis was not put forth as a rigorous model for the biological processes involved and that limitation should perhaps be underscored.

The rationale for selecting the parameters of the "triple-shifted" Rijnmond probit function can be explained as a conservative, qualitative choice to force the function to produce a mortality curve which matches a variety of data from human and animal exposure experience. The consistency of the mortality curve with experience argues for its acceptance as a reasonable estimate of reality.

The weaknesses pointed out by Marshall (1989) are inherent in the probit approach. The amount of data available for hydrogen sulphide exposures is even smaller than for the case of chlorine treated by Marshall. As Marshall states (op. cit., p. 26), a proposed probit function needs to be qualified, as well as quantified. The adjustments to the Rijnmond function which led to the "triple-shifted" function, and the finding by Alberta Public Safety Services that these parameters were consistent with their interpretation of available data are examples of the qualification process which Marshall advocates.

All of the factors which Marshall suggests ought to be incorporated could eventually be addressed with sufficient scientific data and more rigorous models. We do not have these data or models and are unlikely to have them for some time to come. That does not mean that we should not use the probit function to estimate consequences of exposure to hydrogen sulphide, but it does mean that the basis for the parameters used in GASCON2 needs to be reviewed regularly to make sure that the most recent data and concepts are incorporated. The modelling system is constructed so that the probit parameters can be modified easily, as new data are received. If new data suggest that the probit model is fundamentally in error, then the modelling system would have to be revamped.

As Marshall points out, the probit model predicts some fatalities at concentrations less than those which are known to have any measurable effect. It also predicts that there will be some survivors at very high concentrations at which survival is unlikely. These extreme ends of the probit function are very uncertain, and perhaps the limits of applicability should be limited, say, to the L_{01} to L_{99} points or L_{10} to L_{90} points. Either of these choices should have little effect on the overall results of the analysis, which will involve some qualitative choices about the interpretation of the data, in any case. The reality of the possible exposure scenarios needs to be considered. For example, the end of the toxic load curve corresponding to relatively high concentrations persisting for very long exposure times is physically unrealistic.

It must always be kept in mind that the predictions of GASCON2 are semi-quantitative estimates, at best, and that any application of the numbers which GASCON2 produces must be carefully evaluated to incorporate qualifying factors which may be appropriate for a specific application or site.

4.6.3 Fluctuating Load Analysis

The turbulent structure of the atmosphere is responsible for potentially large variations in toxic gas concentration about an average level. Figure 4.14 shows an example of the concentration variability about the average.

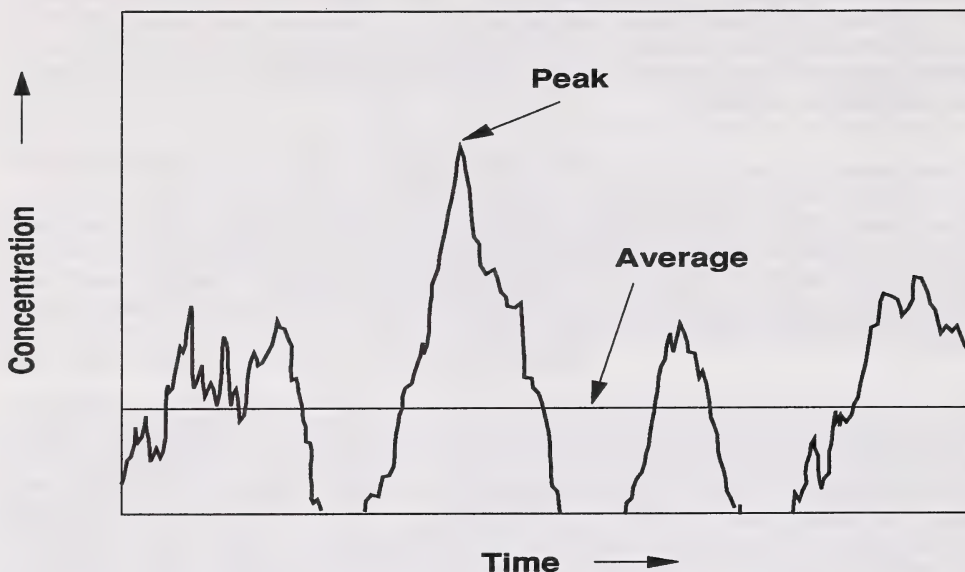


Figure 4.14

Concentration Fluctuations.

Csanady (1973) reports ratios of peak concentrations to average concentrations can be as high as 5, or so. Dispersion models, such as are used in the GASCON2 hazard assessment model (on which the risk is based) can only estimate the average concentration for averaging periods ranging from 3 minutes to a few hours. Since the response of living organisms to toxic gas exposure is highly non-linear, these concentration fluctuations must be accounted for when calculating toxic load and the probability of lethality due to toxic gas exposure.

Fluctuating load analysis is a method whereby the toxic load can be estimated by accounting for concentration fluctuations. It is a development of the work which has been done on modelling concentration fluctuations in plumes (Wilson, 1982; Wilson, 1986; Wilson and Simms, 1985; Wilson *et al.* 1985; Csanady, 1973). Wilson (1987), in an extension to earlier work, has derived a probability density function for the occurrence of toxic load:

$$F(L)dL = \frac{1}{\sqrt{2\pi}LS_L} \exp\left(\frac{-\ln^2\left(\frac{L}{L_m}\right)}{2S_L^2}\right) dL \quad (4.183)$$

This is a log-normal density function, with $F(L)dL$ representing the probability that the toxic load is in the range L to $(L+dL)$. The quantities L_m and S_L are the median toxic load and the toxic load standard deviation, respectively. The closure equations for these two parameters are given in Appendix A. These parameters depend primarily on atmospheric stability which is a measure of the level of turbulence in the atmosphere, and on the height of the toxic gas plume above the ground which strongly influences the average ground-level concentration.

4.7 Model Output

As the name implies, GASCON2 provides estimates of the GAS CONcentrations and CONsequences resulting from a sour gas release.

4.7.1 Concentration

Concentration Profiles

Based on the results of the Passive Dispersion Module, a tabulation of ground-level concentration of H₂S or SO₂ below the plume centreline, as a function of downwind distance from the release site is provided.

For a steady release, the predicted concentration is constant with time. For a transient release, the concentration as a function of time for each downwind position can also be obtained along with the peak concentration predicted for each downwind position.

Hazard Zones

Distances to concentration criteria values (hazard zones) are interpolated from the downwind concentration distance profiles. The user can input up to two concentration criteria for each of two averaging times.

4.7.2 Consequences

Probability of Lethality

The results of the previous sections can be combined to estimate the probability of receiving a lethal toxic load downwind of a given uncontrolled sour gas release event. This probability is the **joint** probability given by:

$$P_L(x, y) = \int_{L=0}^{L=\infty} P(L)F(L)dL \quad (4.184)$$

where: L = Toxic load defined by Equation 4.177 or, more generally, by Equation A.6 (Appendix A).

$P(L)$ = Probability that the toxic load L is lethal as defined by Equation 4.178.

$F(L)dL$ = Probability that the toxic load L is in the range L to $(L + dL)$ as defined by Equation 4.183. In other words, the probability that toxic load L occurs.

$P_L(x,y)$ = Probability of receiving a lethal toxic load L at position (x,y) relative to the sour gas release point $(0,0)$.

The probability $P_L(x,y)$ is a function of the downwind distance x and the crosswind distance y from the sour gas release point since L_M and S_L in Equation 4.183 are also functions of these distances (see Appendix A). The integration indicated by Equation 4.184 is simply the sum of the incremental joint probabilities over the entire range of possible toxic loads, and can be solved analytically using the moment generating function of the lognormal distribution. The result of the integration is a lognormal distribution with a mean and variance which is a function of the means and variances of $P(L)$ and $F(L) dL$.

For a given uncontrolled sour gas release event (emission, geometry and meteorology specified) $P_L(x,y)$ is the individual risk of a person at (x,y) receiving a lethal toxic load. The important inputs to the calculation of $P_L(x,y)$ are:

- location (x,y) ,
- probit parameters $(k_1, k_2, \text{ and } n)$,
- exposure time t_E (for steady releases), and
- concentration of H_2S averaged over t_E minutes.

Potential Fatalities

To estimate the potential number of fatalities (NF) for a given release event, an estimate of the population density in the vicinity of the release site is required. The potential number of fatalities is given by:

$$N_F = \int_{-\infty}^{\infty} \int_0^{\infty} P_L(x,y) D(x,y) dx dy \quad (4.185)$$

where $D(x,y)$ = population density (people/m²).

For this report, a uniform population density of 1 person/Ha has been assumed. This number compares to the average population density for the City of Calgary of 12 people/Ha (City of Calgary, 1987).

The number of potential fatalities N_F is the societal risk for a given uncontrolled sour gas release event. The double integral in Equation 4.185 has infinite limits. In practice, it is only necessary to integrate from the setback distance X_{SB} , out to the distances at which the integrand becomes negligible. In GASCON2, the limits of the integration are determined by user input and it is the responsibility of the user to insure that those limits have afforded an accurate estimate of N_F . It is important to note that estimates of N_F and $P_L(x,y)$ will tend to be conservative (high) since they do not account for the reduction in toxic load which would occur if people were indoors. That is, the model assumes that exposed people are outdoors, directly exposed to the toxic gas plume. Being indoors affords considerable protection for short-term exposure (Purdy *et al.* (1987), Wilson (1980)).

Other Parameters

In addition to $P_L(x,y)$, the GASCON2 model calculates other parameters based on the probit distribution $P(L)$ and the fluctuating load distribution $F(L)$.

The mean toxic load occurring at (x,y) is given in Appendix A as:

$$\bar{L}(x,y) = L_M \exp \left[\frac{S_L^2}{2} \right] \quad (4.186)$$

Expressions for L_M and S_L are also given in Appendix A; they are part of the closure calculation for the fluctuating load distribution.

The probability of the mean toxic load $\bar{L}(x,y)$ being lethal, using Equation 4.178, can be estimated from:

$$P_L(x,y) = \frac{1}{2} \left[1 + \operatorname{erf} \left\{ \frac{k_2 \ln(\bar{L}(x,y)) + k_1 - 5}{\sqrt{2}} \right\} \right] \quad (4.187)$$

Finally, another quantity of interest is the probability of a critical concentration level (χ_L) being exceeded. For this calculation, the concentration fluctuation model of Wilson (1982) is employed:

$$P_E(x) = \frac{\gamma}{2} \left[1 - \operatorname{erf} \left\{ \frac{\ln \left(\frac{\chi_L}{\chi_{MP}} \right)}{\sqrt{2 \ln(1 + i_p^2)}} \right\} \right] \quad (4.188)$$

where:

$$\chi_{MP} = \frac{\bar{\chi}(x)}{\gamma \sqrt{1 + i_p^2}} \quad (4.189)$$

$\bar{\chi}$ is the ensemble average concentration predicted by GASCON2. The peak concentration is used for transient releases. The plume intermittency (γ) and the conditional plume fluctuation intensity (i_p) are defined in Appendix A. Values for these parameters follow from the closure of the fluctuating load calculations indicated in Appendix A. Note that $P_E(x)$ is calculated under the plume centreline only.

4.8 Model Limitations

Before applying any model to solve a specific problem, it is important to recognize the limitations imposed by the model assumptions. The following have been identified as limitations to consider when applying GASCON2:

- *Limited Pipeline Release Scenarios.* GASCON2 can only evaluate End Pipe Ruptures (Figure 2.5) or release scenarios which can be considered as the superposition of two or more End Pipe Rupture cases. For example, the model can evaluate a short rupture located in the middle of a pipeline segment, but not at other locations.
- *Upwind and Downwind Horizontal Jets.* The model cannot evaluate horizontal releases which are oriented at some arbitrary angle to the wind (e.g., crosswind releases).
- *Combustion Module Gas Chemistry.* The chemistry and physics of the ignited plume assume the sour gas to be comprised of methane, carbon dioxide and hydrogen sulphide only. Other gases are accounted for in a limited fashion by the heat of combustion factor. Caution should be exercised in applying the model to sour gas streams (for ignited cases only) whose composition differs significantly from that assumed by the model.
- *No Condensation Effects.* The model does not consider the dispersion and deposition of condensate aerosol clouds. Condensate is defined as a mixture of pentanes and heavier hydrocarbons which exist as a vapour in the formation and a liquid at atmospheric conditions.

The dispersion sub-models incorporate assumptions which can restrict their use to the following conditions:

- *Travel times less than a few hours.* During periods characterized by light winds, disorganized and recirculating wind flows, the usefulness of dispersion models at distances beyond 10 km is limited (Mahoney and Spengler, 1975). A wind speed of 1 m/s (3.6 km/h) and a distance of 10 km corresponds to a travel time of 3 hours.
- *Averaging periods ranging from a few minutes to a few hours.* All the models presented are based on steady state meteorological assumptions (which are typically assumed to exist for either 3 minute to 1 hour periods). For longer averaging periods it is unlikely that the natural variability of the atmosphere will allow a given set of meteorological conditions to persist for periods of more than a few hours.
- *Flat terrain conditions.* Significant topographical features can have blocking, steering, channeling, or deflecting effects on the plume trajectory. The presence of elevated terrain can affect the height of the plume above the ground and can increase the level of turbulence over what would be expected for flat terrain. Moderately rough terrain can be accounted for by using appropriate surface roughness (Z_0) values.

- *Homogeneous terrain.* The models do not address changes in the surface roughness with varying downwind distances. Major surface discontinuities such as the presence of an urban area or large body of water are not addressed. These can produce their own local scale circulation systems. Areas where major surface discontinuities are present may be evaluated by varying the Z_o parameter for different model runs.
- *Steady State Atmospheric Conditions.* The models do not address transient atmospheric phenomena such as the rapid mixing of a plume above the mixing layer by the growth of the mixing height (sometimes called inversion breakup fumigation) or changes in wind direction.

The above mentioned limitations for the Passive Dispersion Module apply to nearly all dispersion models. Many are a result of the inherent uncertainties in describing the behavior of the atmosphere (e.g., *Travel times less than a few hours* and *Averaging periods ranging from a few minutes to a few hours*).

For some cases where a model limitation may be an important factor, some indication of ground level concentrations can be obtained by running the model for different cases which bracket the case to be evaluated. For example the following limitations may be addressed in this manner: *Upwind and Downwind Horizontal Jets, Limited Pipeline Release Scenarios* and *Homogeneous Terrain Conditions*.

The consequences are determined based on the following assumptions:

- *H₂S Lethality.* Consequence estimates are based solely on H₂S inhalation.
- *Population Outdoors and Stationary.* Model assumes population is outdoors and does not flee to the protection of a building.
- *Average Adult Population.* The Probit parameters used represent the average adult population and although they are conservative, they should not be applied to sensitive members of the population.

Models, especially "official" regulatory models, are sometimes extrapolated to conditions beyond those for which the model was developed when no other modelling approaches are available. It is the responsibility of the user to ensure that the models are applied correctly and to note any questionable extrapolations.

5 Model Evaluation

The Model Framework discussed in Section 4 of this report was coded in the FORTRAN computer language and implemented on an MS DOS 80286 personal computer. The formal computer code is referred to as the **GASCON2** (GAS CONcentration and CONsequence) model. Several hundred model runs were made during the development of the model algorithms and computer code to ensure that the code represented the design of the algorithms and behaved as expected based on our understanding of the physics. Once the model code was determined to perform satisfactorily, the following model evaluation exercises were undertaken:

- **Sensitivity Testing.** Selected source and meteorological input parameters were varied within realistic limits to determine the impact on model predictions of ground-level concentrations, distances to critical concentration values, probability of lethalties and potential fatalities (Sections 5.2 to 5.5).
- **Uncertainty Analysis.** An estimation of the inherent and reducible uncertainty associated with model predictions was evaluated. Inherent uncertainty results from the stochastic nature of atmospheric turbulence. Reducible uncertainty results from inadequate physics in the model and from errors in the input parameters (Section 5.6).
- **Comparison of Selected Components.** Selected model components were compared to those employed in other models. The selected components include the transient release rate, plume rise, plume spread and plume dispersion modules (Section 5.7).
- **Comparison With Observations.** Ground-level H₂S and SO₂ predictions were compared to the limited ambient air quality observations available from the Lodgepole, Claresholm and Rainbow Lake sour gas well blowouts (Section 5.8).

5.1 Base Case Conditions

Any modelling system which has the flexibility to address a wide variety of source and meteorological conditions, will have a wide range of possible input parameters. The execution of the sensitivity, uncertainty and comparison exercises require the evaluation of the GASCON2 modelling system with a wide a range of parameters. The definition of source and meteorological base cases which are changed systematically allows the model evaluation to be undertaken in an efficient manner.

5.1.1 Well Blowout

The production capability of gas wells in Alberta is usually expressed in terms of an Absolute Open Flow (AOF) potential. The AOF is an estimated theoretical flow which assumes the pressure at the bottom of the well (sandface) is zero. AOF flow rates vary with the flow characteristics of the geological formation and are typically larger for deeper formations. In Alberta, the larger rates are most likely to occur in the foothills regions.

The surface deliverability of a well will be less than the AOF value due to frictional effects. Table 5.1 compares the surface deliverability (*as a percentage of the AOF*) for a selected typical well and the flow cases depicted in Figure 2.3. The table shows that the tubing has the greatest effect in reducing the surface deliverability for wells which have the highest production capabilities. For wells with a low production capability, the effect of tubing in reducing surface deliverability is minimal.

The values in Table 5.1 were based on the following well conditions:

- Well depth (m) 2660
- Casing inside diameter (mm) 156.3
- Tubing outside diameter (mm) 73.0
- Tubing inside diameter (mm) 62.0
- Reservoir pressure (kPa) 15,900
- Reservoir temperature (°C) 75

Table 5.2 summarizes the *Base Case Emission* scenario for a well release. For the purposes of model evaluation, a base case corresponding to an AOF of $1000 \cdot 10^3 \text{ m}^3/\text{d}$ was selected. The base case further assumes that the well is in the production mode and that the maximum release rate is limited by flow through the tubing ($260 \cdot 10^3 \text{ m}^3/\text{d}$). A further restriction assumes the failure will result in a horizontally oriented jet released in the direction of the wind (Downwind Jet as depicted in Figure 2.4). The presence of a wing valve at the well head was assumed to divert the vertical flow in the tubing to a horizontal release. Wing valves are smaller than the master valves on the wellhead. A wing valve diameter of 52.4 mm was assumed to further restrict the release rate ($240 \cdot 10^3 \text{ m}^3/\text{d}$).

Table 5.1
Surface Deliverability as a Function of Well AOF.

Sandface AOF ($10^3 \text{ m}^3/\text{d}$)*	Casing Flow	Annulus and Tubing Flow	Annulus Flow	Tubing Flow
5000	57.4%	52.2%	39.3%	8.5%
1000	95.0	82.5	76.0	26.0
500	98.0	96.0	92.0	46.0
100	99.0	98.0	97.0	90.0
50	99.2	99.2	99.2	98.6

* At 15 °C and 101.3 kPa.

Table 5.2**Well Blowout Base Case Assumptions.**

Production Phase Subsurface ESD Valves Fail Tubing Flow Downwind Jet	
Sandface AOF ($10^3 \text{ m}^3/\text{d}$)*	1,000
Release Rate ($10^3 \text{ m}^3/\text{d}$)*	240
Release Diameter (mm)	52.4
Gas Temperature ($^{\circ}\text{C}$)	40

* At 15°C and 101.3 kPa.

5.1.2 Pipeline Rupture

Similarly, a wide range of parameters for sour gas pipelines in Alberta is possible. Table 5.3 indicates the range and typical values for sour gas pipelines. For sour gas pipelines located near urban centres, emergency shut down valves (ESD) are located every 2000 to 3000 m to reduce the amount of gas which could be vented to the atmosphere in the event of a rupture. In remote rural settings, a sour gas pipeline may not have any intermediate ESD valves.

Table 5.4 summarizes the *Base Case Emission* scenario selected for a pipeline rupture. The volume of the gas released to the atmosphere was assumed to be 30 percent larger than the volume of gas contained in the ruptured pipeline segment which is isolated from the rest of the system by ESD valves. This 30 percent factor accounts for the additional gas released to the atmosphere during the time required for the ESD valves to respond to the rupture.

Table 5.3**Sour Gas Pipeline Parameters.**

Parameter	Range	Typical
Length (m)	500 to 25,000	2000 to 10,000
Diameter (mm)	60.3 to 610.0	88.9 to 168.3
Maximum Operating Pressure (kPa)	700 to 39,700	3000 to 10,000
Gas Temperature ($^{\circ}\text{C}$)	5 to 45	5 to 45

Table 5.4**Pipeline Rupture Base Case Assumptions.**

End Pipe Rupture All ESD Valves Operate Short Rupture Side Rupture Downwind Jet	
Length (m)	1000
Diameter (mm)	154.1
Pressure (kPa)	5000
Temperature (°C)	30
Friction Factor	0.014
Excess Mass Factor (1+ δ)	1.30
Fractional Hole Size A_E/A_P	1.0

5.1.3 Gas Properties

For the well blowout and the pipeline rupture evaluation, the composition and associated properties of the sour gas are required. It is recognized that sour gas compositions in Alberta represent a wide spectrum of H₂S contents, molecular mass, specific heats and heating values. For the purposes of model evaluation, however, the gas composition and properties given in Table 5.5 were used.

Table 5.5**Gas Composition Base Case Assumptions.**

Composition (Volume Fraction)	
C ₁	0.550
C ₂	0.005
C ₃	0.001
C ₄	0.001
H ₂ S	0.300
CO ₂	0.123
N ₂	0.020
Total	1.000
Molecular Mass (kg/kmole)	25.27
Specific Heat C_p (J/(kg K))	1402
Heat of Combustion (MJ/m ³)*	25.74
Compressibility at Pipeline Conditions	0.83

* Low heat value (15 °C and 101.3 kPa).

5.1.4 Meteorology

Table 5.6 summarizes the *Base Case Meteorology* scenarios used. Two base case meteorology conditions were selected: one for unignited releases and another for ignited releases. The mixing height Z_i , Monin-Obukhov length L and friction velocity U^* values given in the table depend on wind speed and are calculated from the meteorological preprocessor formulations contained in GASCON2.

For the base case well and pipeline release scenarios, minimal plume rises are expected for the unignited case. Experience shows that the maximum predicted hazard zones associated with this type of release tend to occur under low wind speed, stable conditions. For the ignited well release scenario, the buoyancy created by the combusted gases will produce significant plume rise. High wind speed conditions can decrease this rise, producing potential hazard zones larger than those for low wind speed conditions.

Table 5.6
Meteorological Base Case Assumptions.

Stable Conditions	
Surface Roughness Z_o (m)	0.1
Anemometer Height Z_{REF} (m)	10.0
Temperature T_{AO} ($^{\circ}$ C)	0.0
Pressure P_{AO} (kPa)	89.0
Temperature Gradient dT/dZ ($^{\circ}$ C/m)	0.03
Surface Heat Flux H_o (W/m ^{2})	-15.0
Latitude of Site ($^{\circ}$)	51
Unignited Release	
Wind Speed U_{REF} (m/s)	1.0
Mixing Height Z_i (m)	28
Monin-Obukhov Length L (m)	20
Friction Velocity U^* (m/s)	0.06
Ignited Release	
Wind Speed U_{REF} (m/s)	3.0
Mixing Height Z_i (m)	94
Monin-Obukhov Length L (m)	57
Friction Velocity U^* (m/s)	0.22

5.1.5 Modelling Assumptions

Table 5.7 summarizes the assumptions made for the sensitivity testing with respect to the release description and parameters required by the model.

Table 5.7
Model Input Assumptions.

Release Height Z_E (m)	
Well and Surface pipe	1.0
Buried pipe	0.0
Release Angle λ	
Downwind Jet and Cloud	0.0
Vertical	90.0
Upwind	180.0
Drag Coefficient C_D	
Surface facility jet	0.0
Buried pipe jet	2.0
Cloud	3.0
Mach Number at "S" Plane M_s	
Jet	0.30
Cloud	0.01
Added Mass Factor C_M	0.0
Minimum Plume Remaining in Mixed Layer (f)	0.05
Skin Friction with Ground C_F	0.005
Probit Parameters	
k_1	-36.2
k_2	2.366
n	2.5
Average Population Density (people/Ha)	1.0
Set Back Distance from Facility (km)	
Small releases	0.1
Large releases	0.5

The estimation of hazard zones requires the definition of critical concentration values. For the purposes of sensitivity testing, the following concentration criteria were used:

- H₂S 100 ppm as a three-minute average
 20 ppm as a three-minute average
 5 ppm as a one-hour average
 1 ppm as a one-hour average
- SO₂ 1 ppm as a three-hour average

The above "ppm" units refer to the concentration in parts per million by volume. The averaging periods were selected to represent standard meteorology and air quality monitoring times and may not necessarily represent human physiological responses.

5.1.6 Sensitivity Testing

The model sensitivity results are presented in four formats; two for concentrations and two for consequences. The first format is a graphical representation of the ground-level concentration (H₂S or SO₂) below the plume centreline as a function of distance from the release site. The second format is a tabulation of the maximum distances to critical concentration (H₂S or SO₂) values. The concentration-distance profiles help provide a further understanding of the model results and are used to determine the consequences. The third format is a graphical presentation of the individual risk or probability of lethality downwind of a given unignited release scenario. The fourth format is a tabulation of the societal risk or potential number of fatalities for the given H₂S release event.

For the sensitivity analyses, selected well blowout and pipeline rupture scenarios were evaluated for the base case meteorology. These analyses are followed by a sensitivity on selected meteorology parameters for the base case well blowout and pipeline rupture scenarios. For the well blowout evaluations, both unignited (H₂S) and ignited (SO₂) releases are considered. For the pipeline rupture scenario, only unignited releases (H₂S) are considered.

5.2 Well Blowout Source Parameters

Source geometry, flow rate and release angle were selectively changed to observe the effect on predictions.

Exposure Time

Longer exposure times result in lower average concentrations as the crosswind plume spread due to velocity and direction fluctuations increases. For this evaluation of steady state releases, an exposure time of one hour was used for unignited releases and a three hour exposure time was used for ignited releases. The three hour exposure time is assumed to be the limit for a particular set of meteorological conditions. Shorter exposure times result from the early ignition of the escaping sour gas release or the receptor leaving the area. For manned well sites, it is expected that wells would be ignited within an hour.

Figure 5.1 shows the effect of exposure time on downwind concentrations for base case emissions and meteorology. Sixty minute average concentrations are about one half of the 3-minute average concentrations.

The following H₂S concentration profiles for unignited releases are presented as 3-minute averages because emergency response planning is based on the short exposure, high concentration values.

5.2.1 Concentration Profiles

Geometry

Sensitivity analyses were undertaken for the seven well blowout geometry scenarios shown in Table 5.8. Note that the given casing flow rate is assumed to occur through a wing valve, which results in high pressure at the exit. Figures 5.2 and 5.3 show the predicted H₂S and SO₂ concentrations as a function of downwind distance for the release scenarios presented in Table 5.8. From the figures and the associated computer output, the following are noted:

- Horizontal jet releases (Scenarios 1, 3 and 5) result in the largest predicted H₂S concentrations near the well.
- Cloud releases (Scenarios 4 and 7) result in higher H₂S concentrations further downwind of the well.
- Downwind jets (Scenario 1) result in higher H₂S concentrations than upwind jets (Scenario 3). For SO₂ concentrations, these two release geometries result in the same predicted values.
- Larger flow rates associated with the casing (Scenarios 5, 6 and 7) produce higher H₂S but lower SO₂ concentrations than the tubing (Scenarios 1, 2, 3 and 4) for the downwind distances shown.
- Vertical releases (Scenarios 2 and 6) resulted in the lowest H₂S and SO₂ concentrations because of higher plume rise.
- All of the scenarios were modelled as elevated releases except for the upwind jet case which was modelled as a surface release due to its size.
- SO₂ concentrations are not sensitive to source geometry as plume rise is dominated by buoyancy.

Table 5.8

Well Blowout Geometry Sensitivity Scenarios.

Scenario	Flow	Geometry	Release Rate (10 ³ m ³ /d)	Release Diameter (mm)
1	Tubing	Downwind Jet	240	52.4
2	Tubing	Vertical Jet	240	52.4
3	Tubing	Upwind Jet	240	52.4
4	Tubing	Cloud	240	52.4
5	Casing	Downwind Jet	825	52.4
6	Casing	Vertical Jet	825	52.4
7	Casing	Cloud	825	52.4

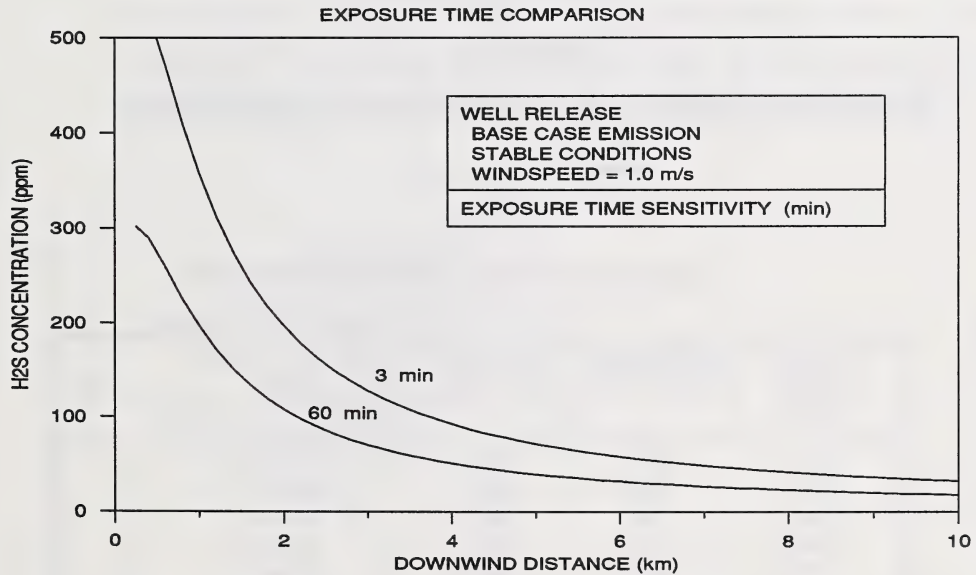


Figure 5.1

**Effect of Exposure Time on Downwind Concentrations
(Base Case Well Blowout and Meteorology).**

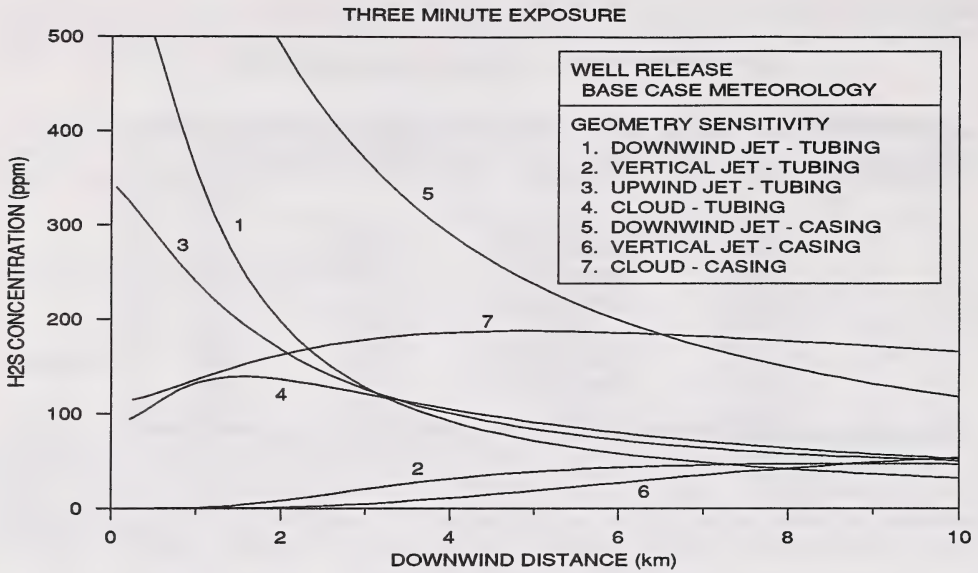


Figure 5.2

Predicted H₂S Concentrations for Selected Well Geometry Scenarios.

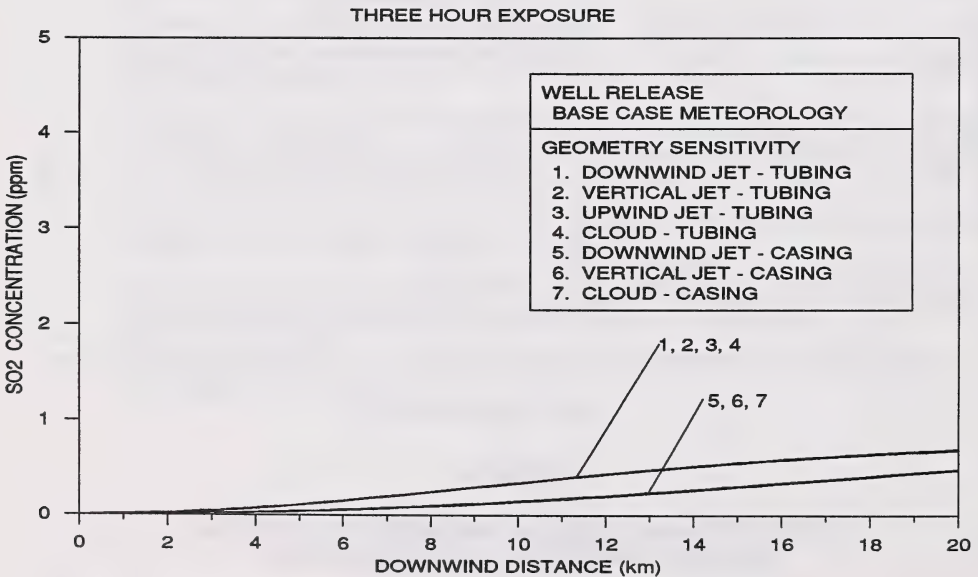


Figure 5.3

Predicted SO₂ Concentrations for Selected Well Geometry Scenarios.

Flow Rate

Sensitivity analyses were undertaken for the six well flow rate scenarios (expressed in terms of well AOF) shown in Table 5.9. The release rate (deliverability) values used are less than the AOF's and are based on the assumptions given in Section 5.1.1. Three of the flow rates are based on tubing flow and three are through the casing. A downwind jet is assumed for each of the flow rates. The release rates shown in Table 5.9 depart from the base case emission given in Table 5.2 in that the horizontal flow is not restricted by the presence of a valve. A horizontal release through a pipe diameter equal to that of the casing may not be a realistic release scenario.

Figures 5.4 and 5.5 show the predicted H₂S and SO₂ concentrations as a function of downwind distance for the flow rate scenarios given in Table 5.9. From the figures and the associated computer output, the following are noted:

- All scenarios were classified as elevated releases.
- The larger the release rate, the larger the predicted H₂S concentrations.
- Larger release rates result in lower predicted SO₂ concentrations near the source.
- The Scenario 1 tubing and Scenario 4 casing release rates are similar. The unignited plume rise associated with casing flow (14 m) is double the rise for tubing flow (7 m) since the casing flow is subsonic, resulting in higher exit temperatures. For the ignited release, the predicted plume rises are nearly identical resulting in similar predicted SO₂ concentrations for the two cases.

Table 5.9

Well Blowout Flow Sensitivity Scenarios.

Scenario	Flow	AOF Rate (10 ³ m ³ /d)	Release Rate (10 ³ m ³ /d)	Release Diameter (mm)
1	Tubing	100	90	62.0
2	Tubing	1000	260	62.0
3	Tubing	5000	425	62.0
4	Casing	100	99	156.3
5	Casing	1000	950	156.3
6	Casing	5000	2870	156.3

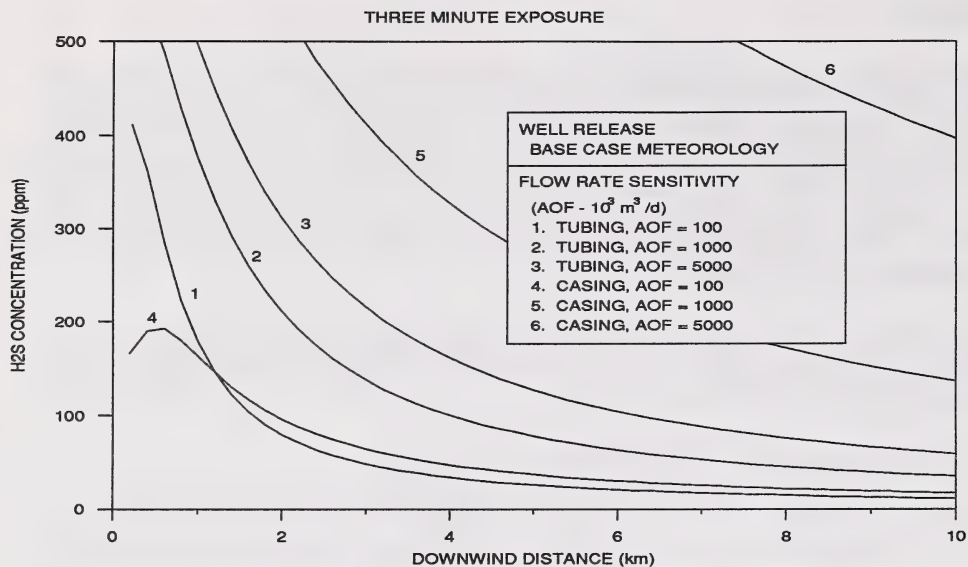


Figure 5.4

Predicted H₂S Concentrations for Selected Well Flow Rates.

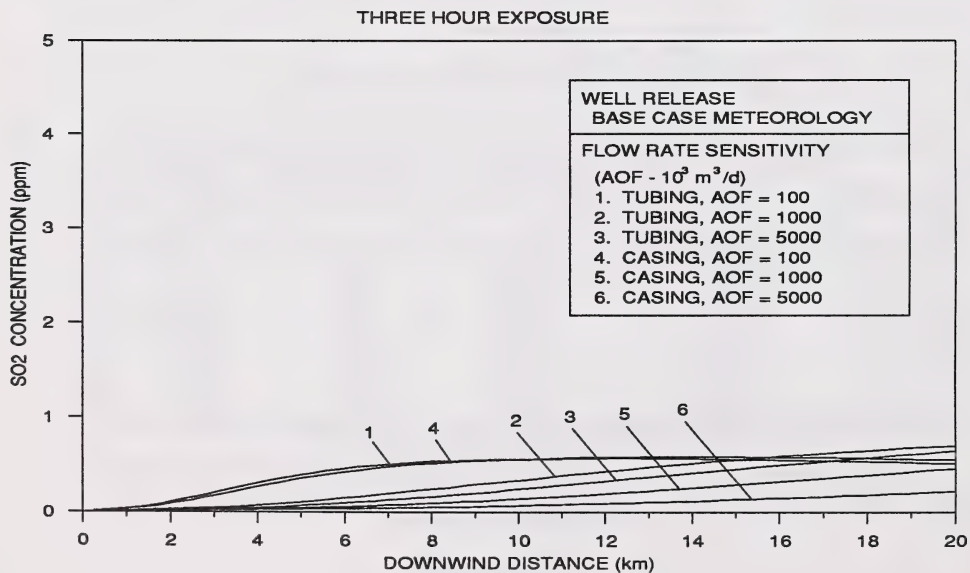


Figure 5.5

Predicted SO₂ Concentrations for Selected Well Flow Rates.

Emission Angle

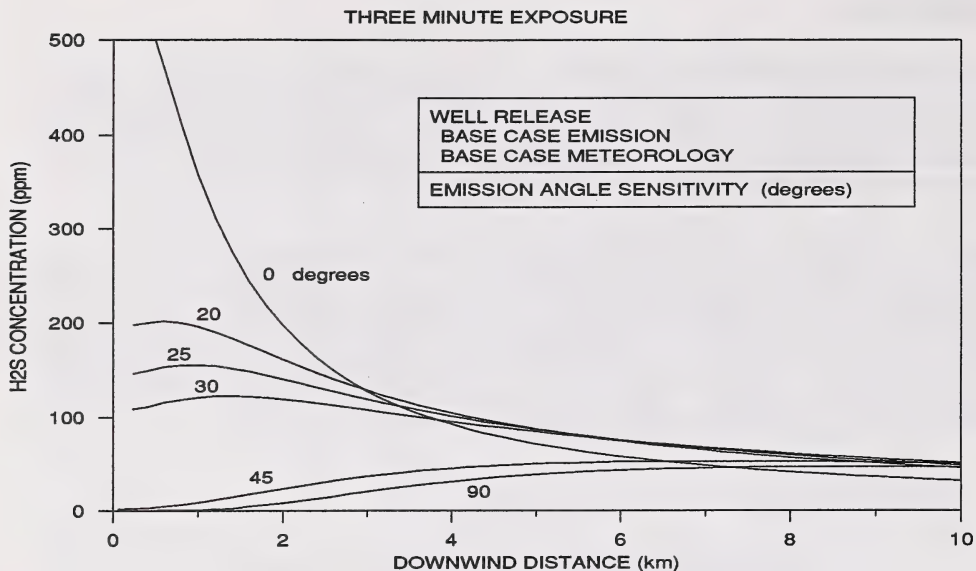
The sensitivity of the predicted H_2S and SO_2 concentrations to the angle of release (emission angle) was undertaken. Recall from Figure 4.2 that a horizontal release corresponds to an emission angle of 0° and a vertical release corresponds to an emission angle of 90° . As the emission angle moves from a vertical ($\lambda = 90^\circ$) release to a horizontal release ($\lambda = 0^\circ$), the momentum component of the plume rise will decrease from a maximum value to zero.

Figures 5.6 and 5.7 show the emission angle sensitivity of the predicted H_2S and SO_2 concentrations, respectively. The more vertical the emission angle (larger λ), the smaller the predicted H_2S concentrations near the well. H_2S concentrations approach the same level further downwind. SO_2 concentrations are not sensitive to the emission angle. As illustrated in Table 5.10, the emission angle (λ) affects the final plume height (Z_{PF}) for unignited releases but not for ignited releases. Plume rise for ignited releases is dominated by buoyancy considerations. All scenarios were classified as elevated releases.

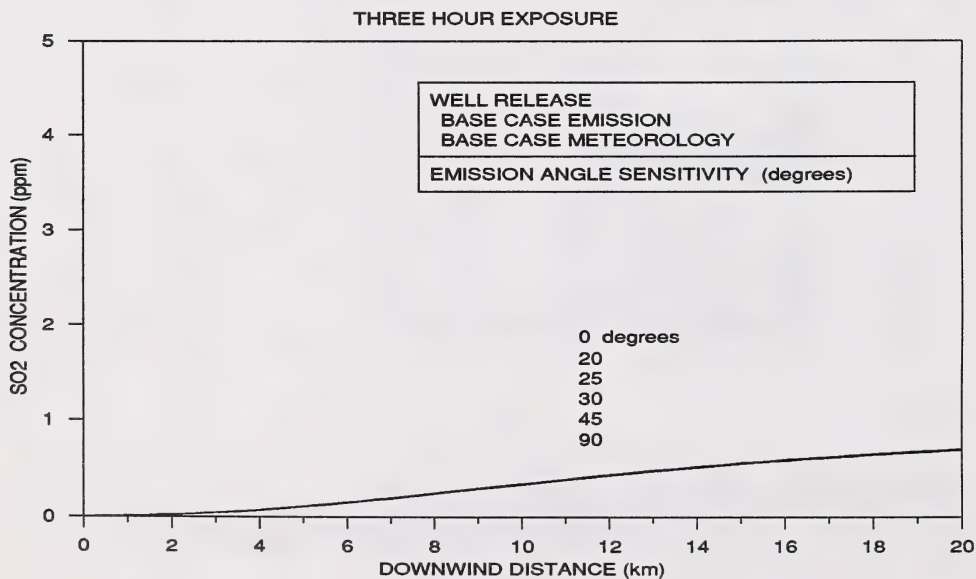
Table 5.10

Well Blowout Emission Angle Sensitivity Scenarios.

Scenario	λ (degrees)	Z_{PF} (m)
Unignited	0	9
	20	19
	25	21
	30	23
	45	31
	90	32
Ignited	0	109
	20	109
	25	109
	30	109
	45	109
	90	109



Predicted H₂S Concentrations for Selected Emission Angles.



Predicted SO₂ Concentrations for Selected Emission Angles.

5.2.2 Hazard Zones

Table 5.11 summarizes the hazard zones associated with well blowout sensitivity runs. The largest hazard zones are associated with horizontally directed releases and large flow rates. Hazard zones greater than 10 km were not shown in Table 5.11.

For the unignited release where the base case meteorology assumes a wind speed of 1 m/s, the largest hazard zones are much greater than 10 km. These distances correspond to plume travel times beyond 3 hours. The large predicted zones associated with these travel times are not presented as it is unlikely that a given meteorological condition will persist for this period of time due to the natural variability of the atmosphere.

For low wind speed stable conditions, large horizontal plume meandering will increase the effective dispersion of a plume for averaging times larger than half an hour (approximate). This factor has not been accounted for in the model, and as a consequence, the model which assumes steady state meteorological conditions, will likely predict larger hazard zones (based on one and three hour averaging times) than expected. For a three-minute averaging time, the plume meander is not expected to significantly affect the predicted hazard zone values given in the table.

At the larger downwind distances, small changes in an input parameter can cause larger changes in the predicted hazard zone than at the smaller distances. This is due to the relatively "flat" nature of the concentration-downwind distance profile at large distances. At small distances, the profile is relatively "steep" and small changes in an input parameter will also produce small changes in the predicted hazard zones.

Table 5.11

**Hazard Zone Sensitivity to Well Blowout Parameters
(Base Case Meteorology).**

Distance (km) to:						
Case		3 minute H ₂ S		1 hour H ₂ S		3 hour SO ₂
		100 ppm	20 ppm	5 ppm	1 ppm	1 ppm
Tubing	Downwind Jet	3.7	> 10	> 10	> 10	0
	Vertical Jet	0	> 10	> 10	> 10	0
	Upwind Jet	4.0	> 10	> 10	> 10	0
	Cloud	4.3	> 10	> 10	> 10	0
Casing	Downwind Jet	> 10	> 10	> 10	> 10	0
	Vertical Jet	0	> 10	> 10	> 10	0
	Cloud	> 10	> 10	> 10	> 10	0
Tubing	90•10 ³ m ³ /d	1.7	6.2	> 10	> 10	0
	260•10 ³ m ³ /d	4.0	> 10	> 10	> 10	0
	425•10 ³ m ³ /d	6.2	> 10	> 10	> 10	0
Casing	99•10 ³ m ³ /d	1.9	8.6	> 10	> 10	0
	950•10 ³ m ³ /d	> 10	> 10	> 10	> 10	0
	2870•10 ³ m ³ /d	> 10	> 10	> 10	> 10	0
Angle	0° (Downwind)	3.7	> 10	> 10	> 10	0
	20°	4.2	> 10	> 10	> 10	0
	25°	4.1	> 10	> 10	> 10	0
	30°	3.6	> 10	> 10	> 10	0
	45°	0	> 10	> 10	> 10	0
	90° (Vertical)	0	> 10	> 10	> 10	0

5.2.3 Probability of Lethality

Exposure Time

Sensitivity analyses were undertaken to examine the influence of exposure time on the predicted lethality for steady-state well releases. The base case well emission and base case meteorology were used.

Exposure times of 3 hour, 1 hour, 30 minutes and 3 minutes were evaluated. Figure 5.8 shows the effect of exposure time on the lethality curves. The longer the exposure time, the higher the probability of receiving a lethal toxic load.

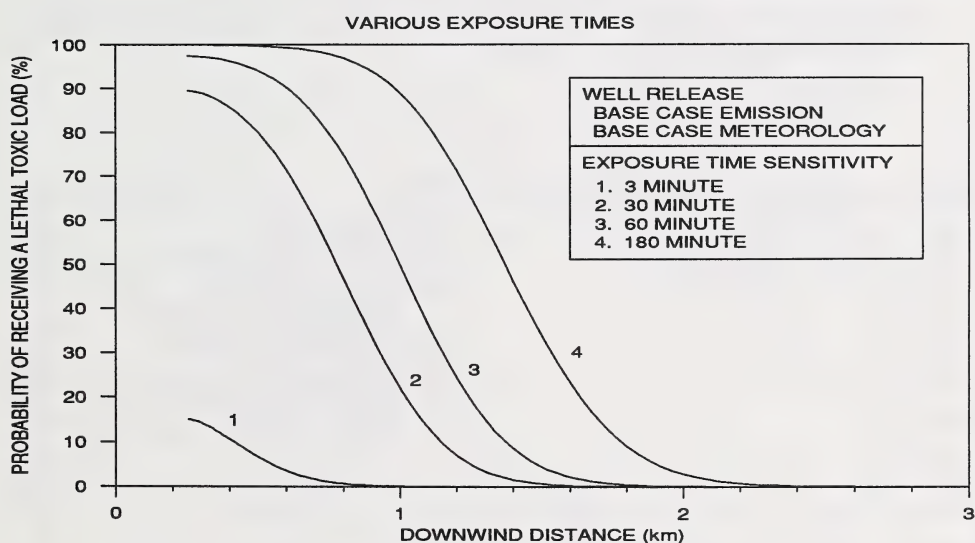


Figure 5.8

**Predicted Lethality Sensitivity to Exposure Time
(Base Case Well Blowout and Meteorology).**

Geometry

Table 5.8 showed seven well blowout geometry scenarios for which a sensitivity analysis was undertaken. Figure 5.9 shows the graph of probability of lethality under the plume centreline versus downwind distance for these seven geometries. From the figure and the associated computer output, the following are noted:

- Only horizontal jets (Scenarios 1, 3 and 5) result in significant probabilities of lethality.
- Downwind jets (Scenario 1) result in larger probabilities than upwind jets (Scenario 3).
- Larger flow rate downwind jets (Scenario 5, casing flow) produce larger probabilities than smaller flow rate downwind jets (Scenario 1, tubing jet).
- Vertical releases (Scenarios 2 and 6) resulted in low H_2S concentrations due to high plume rise, and hence the probability of lethality is very low.
- High plume rise of cloud releases (Scenarios 4 and 7) gave low H_2S concentrations and hence low probabilities of lethality.

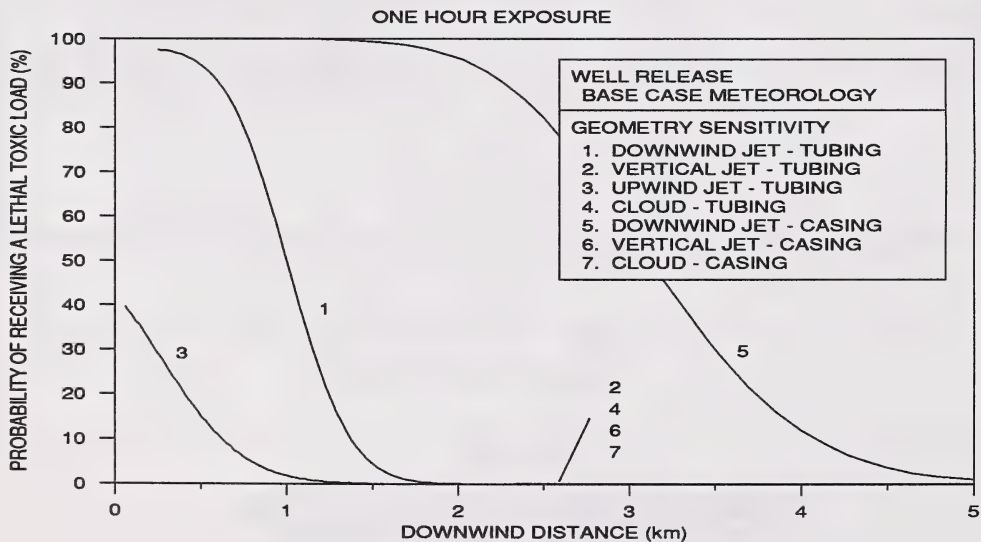


Figure 5.9

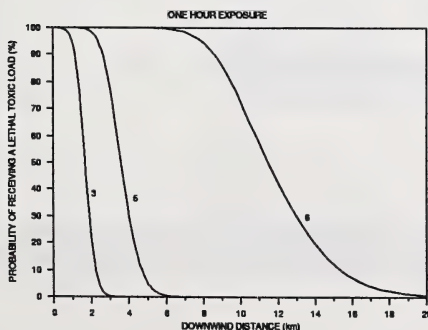
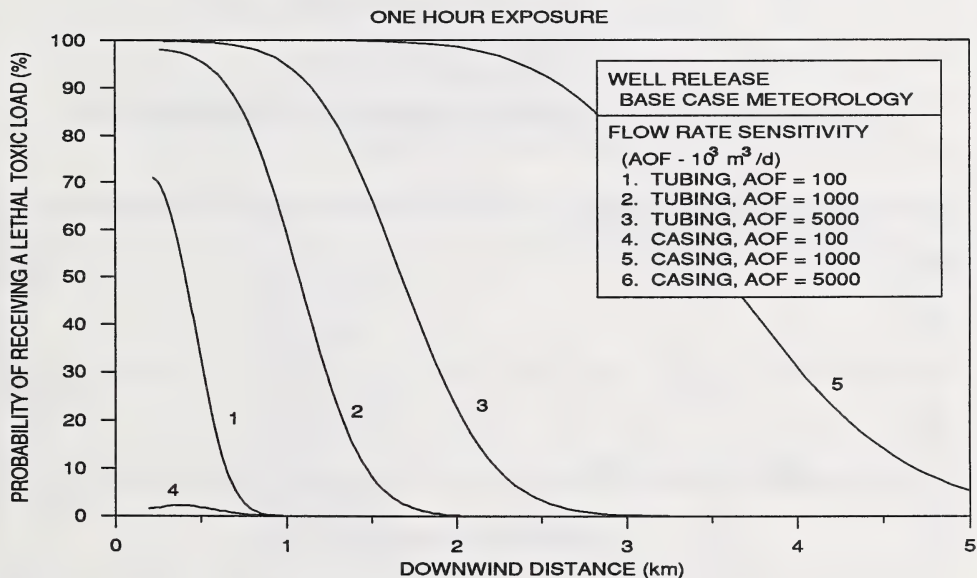
Predicted Lethality for Selected Well Geometry Scenarios.

Flow Rate

Six well flow rate scenarios were shown in Table 5.9. A downwind jet is assumed for each of the flow rates, and the flows are not restricted by the presence of a valve fitting. A horizontal release through a pipe diameter equal to that of the casing may not be a realistic release scenario.

Figure 5.10 shows the lethality curves for these six flow rate scenarios; from the figure and the associated computer output, the following is noted:

- The larger the release rate, the higher the probability of lethality.
- Although Scenario 1 and Scenario 4 have similar release rates, the casing flow is predicted to rise further and, hence, to give smaller H_2S concentrations and a smaller probability of lethality.



Expanded Distance Scale.

Figure 5.10
Predicted Lethality for
Selected Well Flow Rates.

Emission Angle

The sensitivity of the probability of lethality to the angle of release was undertaken. An emission angle of 0° corresponds to a horizontal release (downwind jet); and angle of 90° to a vertical release (vertical jet). Table 5.10 showed the emission angles considered in this sensitivity test, as well as the final plume height.

Figure 5.11 shows the lethality curves corresponding to the different emission angles. For the base case emission and base case meteorology, emission angles greater than 20° or so result in negligible probability of lethality. The largest probabilities result from horizontal releases (downwind jets).

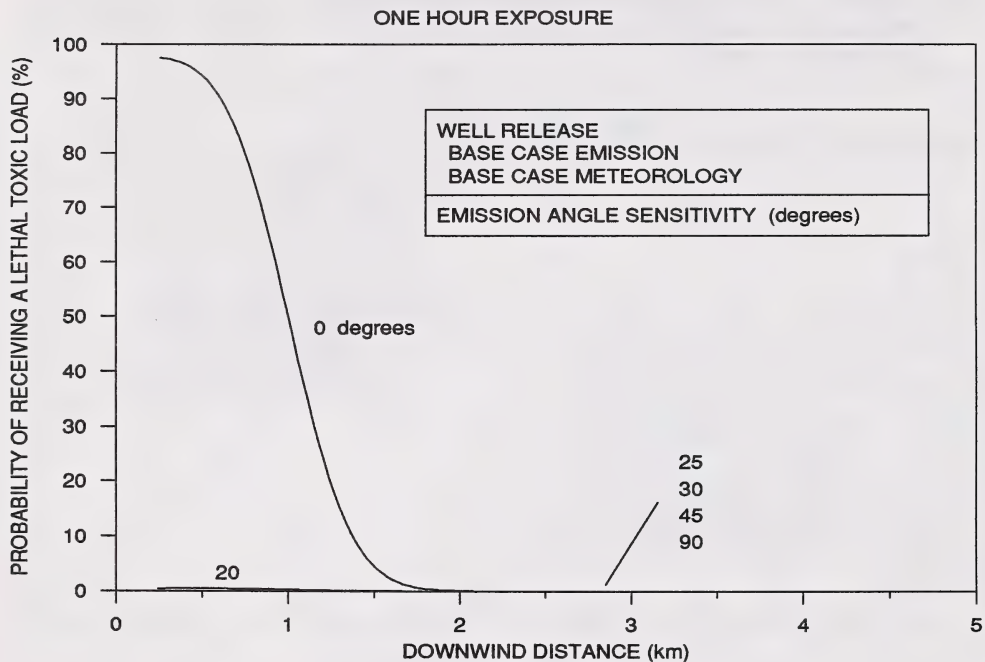


Figure 5.11

Predicted Lethality for Selected Emission Angles.

5.2.4 Potential Fatalities

Table 5.12 shows the potential number of fatalities corresponding to the various exposure times for the base case emission and meteorology. The longer an area is exposed to an unignited release, the higher the potential fatalities.

Table 5.13 summarizes the potential number of fatalities associated with the well blowout sensitivity runs. Horizontally directed releases and large flow rates result in the largest potential number of fatalities. The largest potential number of fatalities is associated with horizontal casing flow, for which significant probabilities of lethality extend up to 20 km

or so downwind of the release. Since the base case meteorology assumes a wind speed of 1 m/s for stable conditions, this amounts to a 5.5 hour travel time, which is beyond the limit that one would assume for persistence of any meteorological condition.

Table 5.12

**Potential Number of Fatalities Sensitivity to Exposure Time
(Base Case Well Blowout and Meteorology).**

Exposure Time	Potential Number of Fatalities
3-minute	0.2
30-minute	3
1-hour	5
3-hour	9

Table 5.13

**Potential Number of Fatalities Sensitivity to Well Blowout Parameters
(Base Case Meteorology).**

	Case	Potential Number of Fatalities
Tubing	Downwind Jet	5
	Vertical Jet	0
	Upwind Jet	1
	Cloud	0
Casing	Downwind Jet	29
	Vertical Jet	0
	Cloud	0
Tubing	90•10 ³ m ³ /d	1
	260•10 ³ m ³ /d	6
	425•10 ³ m ³ /d	12
Casing	99•10 ³ m ³ /d	0
	950•10 ³ m ³ /d	37
	2870•10 ³ m ³ /d	247
Angle	0° (Downwind)	5
	20°	0
	25°	0
	30°	0
	45°	0
	90° (Vertical)	0

5.3 Well Blowout Meteorology Parameters

For the base case well blowout release scenario, the model sensitivity was evaluated for the selected meteorology parameters given in Table 5.14. Base case conditions are shown in bold face. The model default vertical temperature gradients of 0.03, -0.01 and -0.015 °C/m were assumed for stable, neutral and unstable conditions, respectively. These correspond to vertical *potential* temperature gradients of 0.04, 0.00 and -0.005 °C/m respectively.

Table 5.14

Well Blowout Meteorology Sensitivity Parameters.

Surface Roughness	Z_o (m)	0.1 0.3 1.0
Ambient Temperature	T_A (°C)	-20 0 20
Stable Conditions		
Wind Speed	U_{REF} (m/s)	1 2 3 5
Neutral Conditions		
Wind Speed	U_{REF} (m/s)	1 2 3 5 10 15
Unstable Conditions		
Wind Speed	U_{REF} (m/s)	1 2 3

5.3.1 Concentration Profiles

Surface Roughness

Sensitivity analyses about the base case meteorology were undertaken for three surface roughness values. Examples of terrain types corresponding to these selected values of surface roughness are:

- $Z_o = 0.1$ m Flat or gently rolling terrain covered by mature agricultural crops with scattered wind breaks and farm buildings.
- $Z_o = 0.3$ m Flat or gently rolling terrain with continuous residential development.
- $Z_o = 1.0$ m Flat or gently rolling terrain covered with obstructions several tens of metres in height (e.g., forests or downtown urban areas).

Figures 5.12 and 5.13 show the predicted H_2S and SO_2 concentrations as a function of downwind distance and surface roughness. The predicted H_2S and SO_2 concentration profiles are sensitive to the surface roughness. For surface roughnesses of 0.3 and 1.0 m the unignited releases are modelled as surface releases. Larger values of surface roughness result in increased SO_2 concentrations near the well but decreased H_2S concentrations near the well. Smaller values of surface roughness are associated with smaller values of mixing height (Z_i) which decreases plume spread (σ_y and σ_z) for a given plume height.

Table 5.15 illustrates the change in PBL parameters associated with the change in Z_o values. The last case presented in the table is not applicable to a stable atmosphere since, according to the model definition of stability, the wind shear is assumed to overcome the thermal stability when L is greater than 500 m. For this reason, the corresponding curve ($Z_o = 1.0$ m) was not shown on Figure 5.13.

Table 5.15
PBL Parameter Sensitivity to Surface Roughness
for Stable Conditions.

Z_o (m)	U_{REF} (m/s)	Z_i (m)	U^* (m/s)	L (m)
0.1	1.0	28	0.058	20
0.3	1.0	37	0.076	27
1.0	1.0	56	0.116	41
0.1	3.0	95	0.221	57
0.3	3.0	183	0.317	169
1.0 ^a	3.0	922	0.521	750

a - not applicable to stable conditions, reclassified as neutral

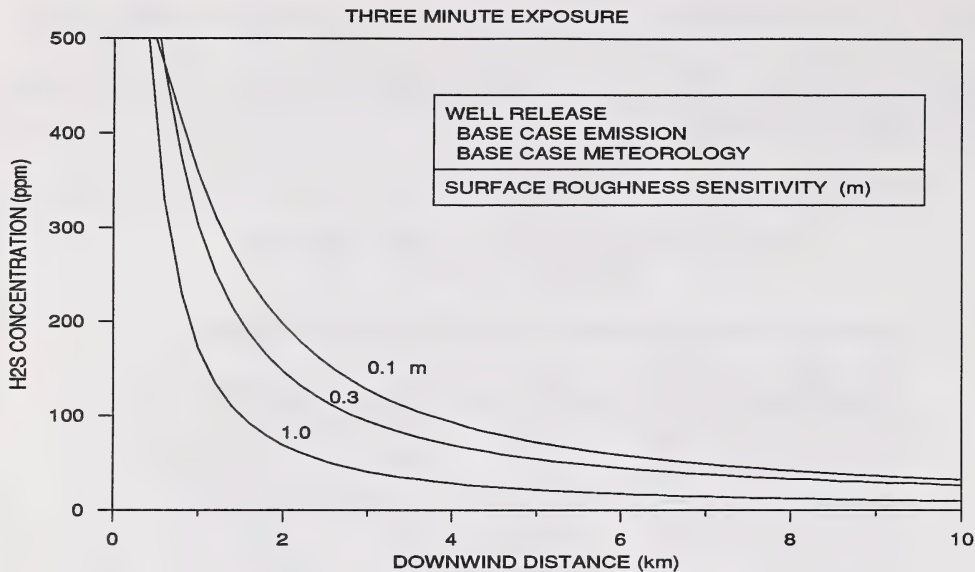


Figure 5.12

Predicted H₂S Concentrations for Selected Surface Roughness Values.

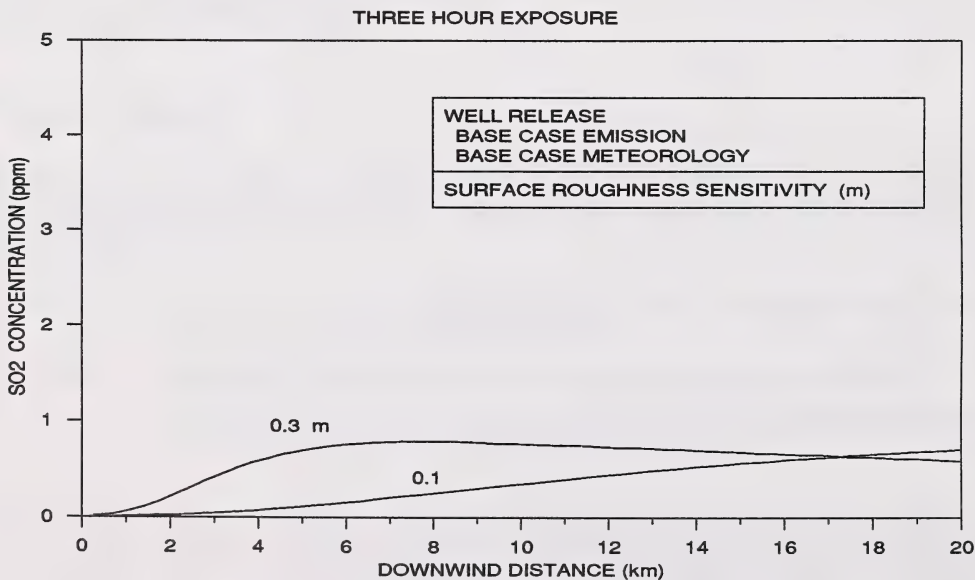


Figure 5.13

**Predicted SO₂ Concentrations for Selected Surface Roughness Values
(Z₀ = 1.0 m Curve Not Shown; See Text for Explanation).**

Ambient Temperature

Sensitivity analyses about the base case meteorology were undertaken for three ambient temperature values. Figures 5.14 and 5.15 show the predicted H₂S and SO₂ concentrations as a function of downwind distance and ambient temperatures (T_{AO}). Larger ambient H₂S concentrations are associated with higher ambient temperatures.

For the horizontal jet releases considered in the base case, the plume rise is due to buoyancy effects. The higher the ambient temperature, the smaller the difference in density between the escaping gases and the ambient air. The lower density results in a decreased plume rise which increases the resultant ambient concentrations. Table 5.16 illustrates the change in plume height (Z_{PF}) for the different temperatures. Note that the 20 °C case was classified as a surface release and the 0 and -20 °C cases were classified as elevated releases.

For the ignited case, the plume rise is not very sensitive to ambient temperature variations. Although the buoyancy flux increases, the plume rise decreases with decreasing ambient temperature. This is due to sensitivity of the method used to calculate buoyant plume rise to the Brunt-Vaisala frequency S_o which depends on $Z_C (= L_C + L_S \sin \lambda)$, the elevation of the "C" plane.

Table 5.16

Plume Height Sensitivity to Ambient Temperature.

Case	T_{AO} (°C)	Z_{PF} (m)
Unignited	20	7
	0	9
	-20	11
Ignited	20	111
	0	109
	-20	106

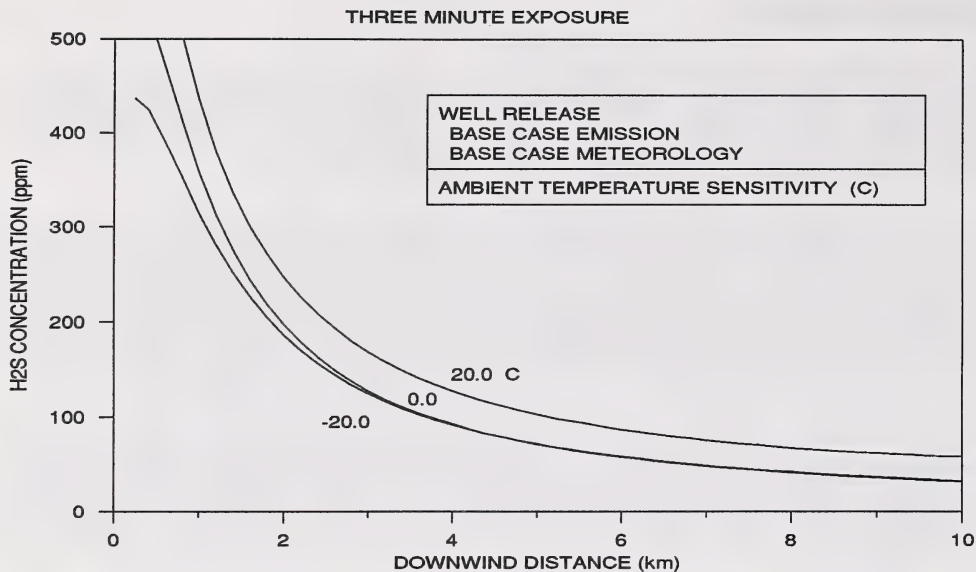


Figure 5.14

Predicted H₂S Concentrations for Selected Ambient Temperatures.

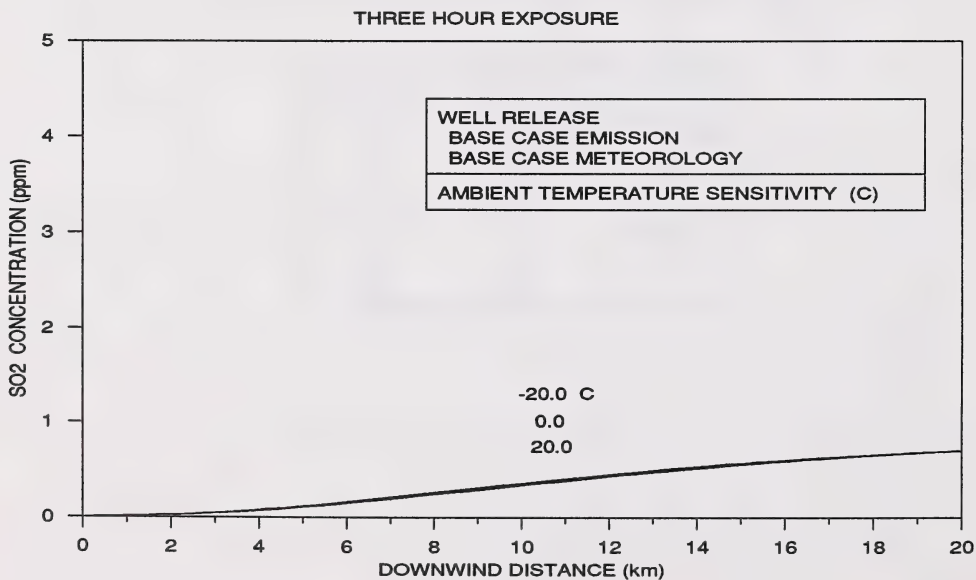


Figure 5.15

Predicted SO₂ Concentrations for Selected Ambient Temperatures.

Stable Conditions

For stable conditions ($H_O = -15 \text{ W/m}^2$), sensitivity analyses were undertaken with four wind speed values. Figures 5.16 and 5.17 show the predicted H_2S and SO_2 concentrations as a function of downwind distance and wind speed (U_{REF}). For the unignited case, the maximum H_2S concentration occurs with a wind speed of 1 m/s. For the ignited case, the maximum SO_2 concentration occurs with a wind speed of 5 m/s.

Wind speed affects the predicted PBL parameters, the plume rise and the along wind dilution. Table 5.17 illustrates some of these points. In particular, as the wind speed increases, the following are noted:

- Wind shear generated mixing height (Z_i) increases,
- Friction velocity (U^*) increases,
- Monin-Obukhov length (L) increases,
- Unignited plume height (Z_{PF}) decreases, and
- Ignited plume height (Z_{PF}) decreases.

Table 5.17

PBL Parameter Sensitivity for Stable Conditions.

U_{REF} (m/s)	Z_i (m)	U^* (m/s)	L (m)	Unignited		Ignited	
				Z_{PF} (m)	f (%)	Z_{PF} (m)	f (%)
1	28	0.058	20	9	100	148	100
2	42	0.116	20	8	100	122	100
3	95	0.221	57	8	100	109	100
5	306	0.424	402	8	100	94	100

Unlimited mixing is assumed under stable conditions, thus f is constant ($f = 100\%$). If plume rise Z_{PF} exceeds the boundary layer height Z_i , the plume spreads are set to a minimum value. All of the scenarios were classified as elevated releases.

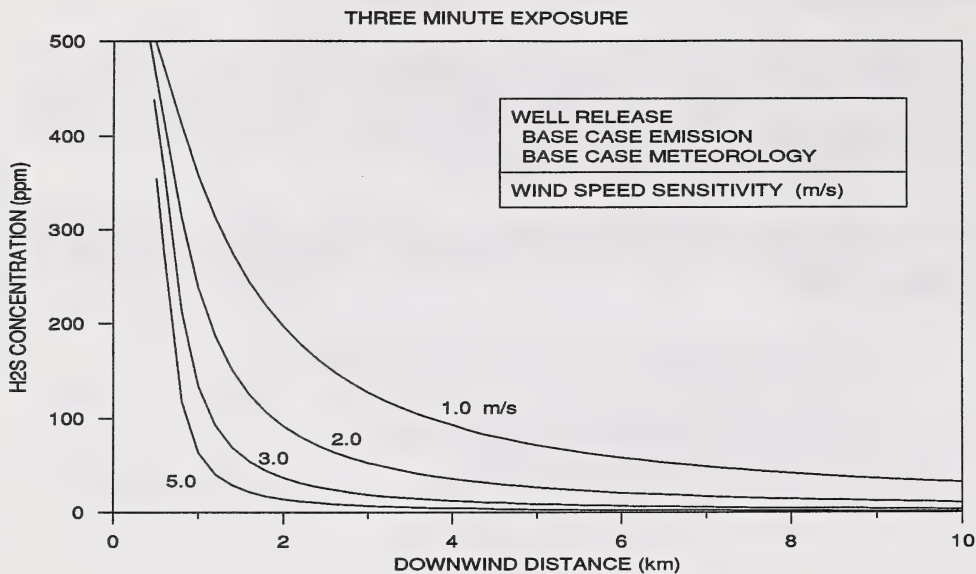


Figure 5.16

Predicted H₂S Concentrations for Selected Wind Speeds (Stable Conditions).

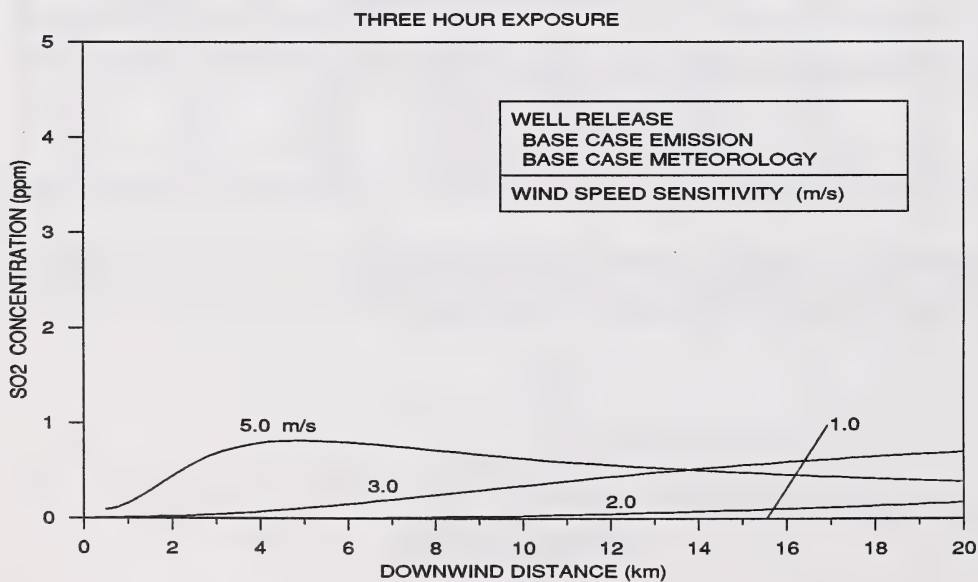


Figure 5.17

Predicted SO₂ Concentrations for Selected Wind Speeds (Stable Conditions).

Neutral Conditions

For neutral conditions, sensitivity analyses were undertaken with six wind speed values assuming a surface heat flux (H_0) of -5 W/m^2 . Figures 5.18 and 5.19 show the predicted H_2S and SO_2 concentrations as a function of downwind distance and wind speed (U_{REF}). For the unignited case, the maximum H_2S concentration occurs with a wind speed of 3 m/s; for the ignited case the maximum SO_2 concentration occurs with high wind speeds (10 to 15 m/s).

As in stable conditions, wind speed also affects the predicted PBL parameters, the plume rise and the along wind dilution. For a given release, a secondary influence also involves the plume penetration factor. Table 5.18 illustrates some of these points. In particular, as the wind speed increases, the following are noted:

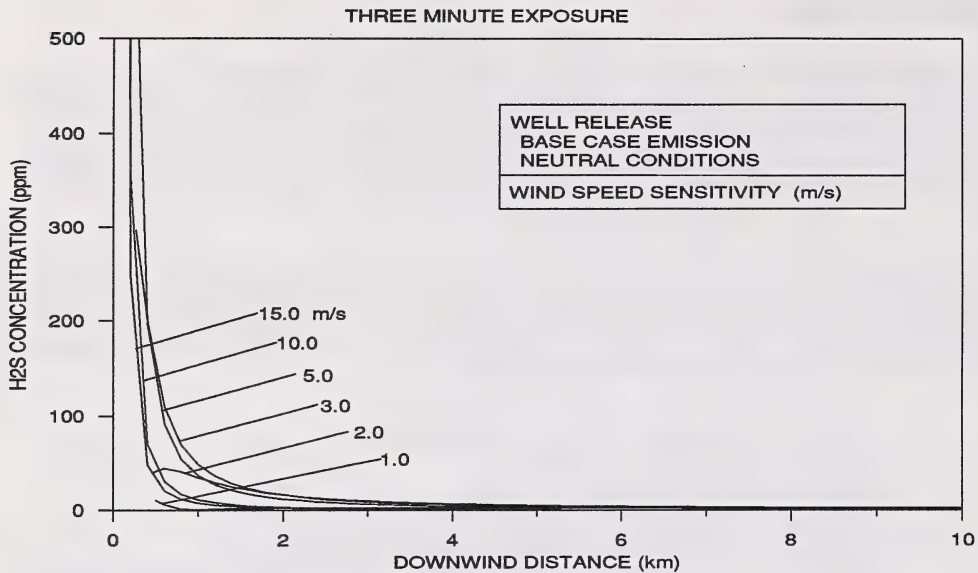
- Wind shear generated mixing height (Z_i) increases,
- Friction velocity (U^*) increases,
- Monin-Obukhov length (L) increases,
- Unignited plume height (Z_{PF}) decreases,
- Ignited plume height (Z_{PF}) increases and then decreases, and
- Percent of ignited and unignited plumes remaining in the mixed layer (f) increases.

Table 5.18

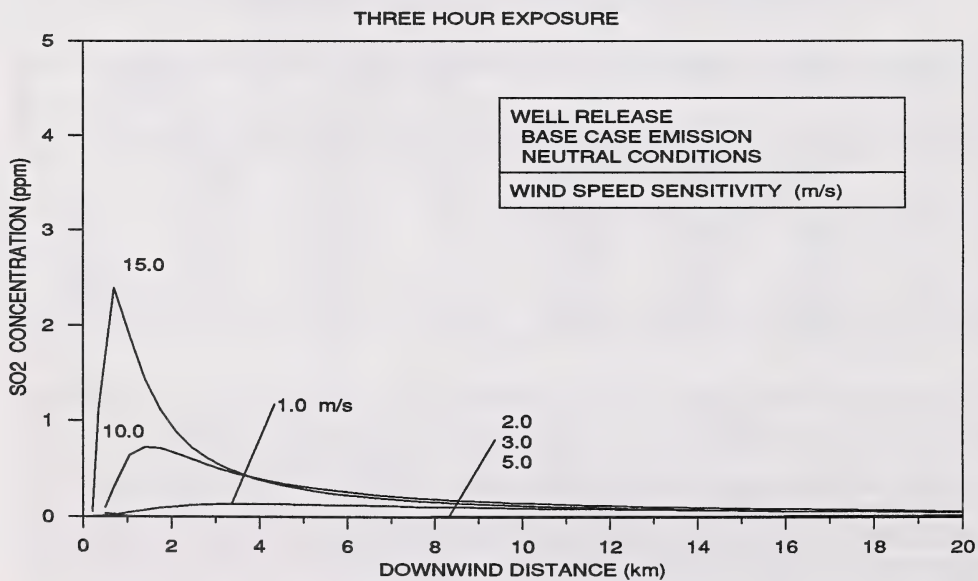
PBL Parameter Sensitivity for Neutral Conditions.

U_{REF} (m/s)	Z_i (m)	U^* (m/s)	L (m)	Unignited		Ignited	
				Z_{PF} (m)	f (%)	Z_{PF} (m)	f (%)
1	154	0.087	10	123	37	154	5
2	307	0.174	83	41	100	307	5
3	461	0.261	281	15	100	406	21
5	768	0.434	1301	5	100	431	100
10	1537	0.869	10411	2	100	79	100
15	2305	1.303	35138	1	100	42	100

For the unignited case (Figure 5.18), the behavior of the low wind speed concentration profiles requires an explanation. For a wind speed of 1 m/s, when the plume reaches its final rise, only 37% of the plume remains in the mixing layer resulting in near zero concentrations at large downwind distances. For a wind speed of 2 m/s, competing effects between the rise and dilution cause the concentration profile to decrease when final rise is reached. For wind speeds greater than 3 m/s, turbulence dominates the profiles which result in concentrations being inversely proportional to the wind speed. At wind speeds of 5 and 10 m/s, the final rise is less than 5 m and these scenarios are modelled as surface releases.



Predicted H₂S Concentrations for Selected Wind Speeds (Neutral Conditions).



Predicted SO₂ Concentrations for Selected Wind Speeds (Neutral Conditions).

The ignited plume (Figure 5.19) exhibits the normally expected behavior of having the plume height decrease with increasing wind speed for wind speeds greater than 2 m/s. For low wind speeds, the plume rise for the ignited portion of the plume remaining within the mixed layer is limited by the mixing height and a large portion of the plume penetrates through the top of the mixing layer ($f \sim 5\%$). As the wind speed increases, more and more of the ignited plume remains in the mixed layer since the mixing height and plume bend-over increases.

Unstable Conditions

For unstable conditions, sensitivity analyses were undertaken with three wind speed values assuming a surface heat flux (H_o) of 50 W/m² and a mixing height (Z_i) of 100 m. Figures 5.20 and 5.21 show the predicted H₂S and SO₂ concentrations as a function of downwind distance and wind speed (U_{REF}). For the unignited case, the maximum H₂S concentrations occurs with a wind speed of 3 m/s. For the ignited case, the maximum SO₂ concentration occurs with a wind speed of 2 m/s.

The value for the convective velocity scale (W^*) associated with the selected unstable condition is 0.542 m/s. According to the model definition of stability, neutral conditions should be assumed for wind speeds greater than 3.2 m/s ($U_{REF} = 6 W^*$). Wind speed affects the predicted PBL parameters, the plume rise and the along wind dilution. For a given release, a secondary influence involves the plume penetration factor. Table 5.19 illustrates some of these points.

As the wind speed increases, the following are noted:

- Friction velocity (U^*) increases,
- Monin-Obukhov length (L) decreases (becomes more negative),
- Unignited plume height (Z_{PF}) decreases,
- Ignited plume height (Z_{PF}) remains constant, and
- Percent of ignited plume remaining in the mixed layer (f) increases.

The unignited plume remains in the mixing layer ($f = 100\%$) for all wind speeds and, as a consequence, exhibits the normally expected behavior of having the plume height decrease with increasing wind speed. For the ignited plume, the plume rise is limited by the mixing height and when the vertical plume spread σ_z exceeds 1.6 Z_i with uniform mixing in the vertical direction assumed.

Table 5.19

PBL Parameter Sensitivity for Unstable Conditions.

U_{REF} (m/s)	U^* (m/s)	L (m)	Unignited		Ignited	
			Z_{PF} (m)	f (%)	Z_{PF} (m)	f (%)
1	0.134	-4	58	100	100	55
2	0.214	-16	40	100	100	100
3	0.293	-40	32	100	100	100

Further sensitivity runs were undertaken for unstable conditions to evaluate the effect of varying the mixing height (Z_i) and the surface heat flux (H_o) (Table 5.20). Note that the ignited case ($U_{REF} = 3$ m/s, $H_o = 50$ W/m² and $Z_i = 50$ m) presented in Table 5.20 is not applicable to unstable conditions since according to the model definition of stability, neutral conditions should be assumed for wind speeds greater than 2.6 m/s ($U_{REF} = 6$ W*). The same also applies for the ignited case ($U_{REF} = 3$ m/s, $H_o = 10$ W/m² and $Z_i = 100$ m) since neutral conditions should be assumed for wind speeds greater than 1.9 m/s ($U_{REF} = 6$ W*). From Table 5.20, we can note:

- Small values of Z_i can restrict the plume rise for the unignited scenarios,
- Relatively large values for Z_i can restrict the plume rise for the ignited scenarios,
- For a given Z_i (100 m), as H_o increases, W^* increases and the plume height (Z_{PF}) decreases for the unignited scenarios,
- For a given Z_i (100 m), H_o has no effect on the plume height (Z_{PF}) if the rise is limited by Z_i .

For unstable conditions, the presence of an additional independent PBL parameter increases the complexity of evaluating dispersion.

Table 5.20

PBL Parameter Sensitivity for Z_i and H_o (Unstable Conditions).

H_o (W/m ²)	Z_i (m)	W^* (m/s)	Unignited $U_{REF} = 1$ m/s		Ignited $U_{REF} = 3$ m/s	
			Z_{PF} (m)	f (%)	Z_{PF} (m)	f (%)
50	50	0.430	50	100	406 ^a	21
50	100	0.542	58	100	100	100
50	500	0.928	58	100	500	100
50	1000	1.173	58	100	672	100
10	100	0.317	100	100	406 ^a	21
50	100	0.542	58	100	100	100
100	100	0.682	45	100	100	100
150	100	0.781	39	100	100	100

a - not applicable to unstable conditions, reclassified as neutral.

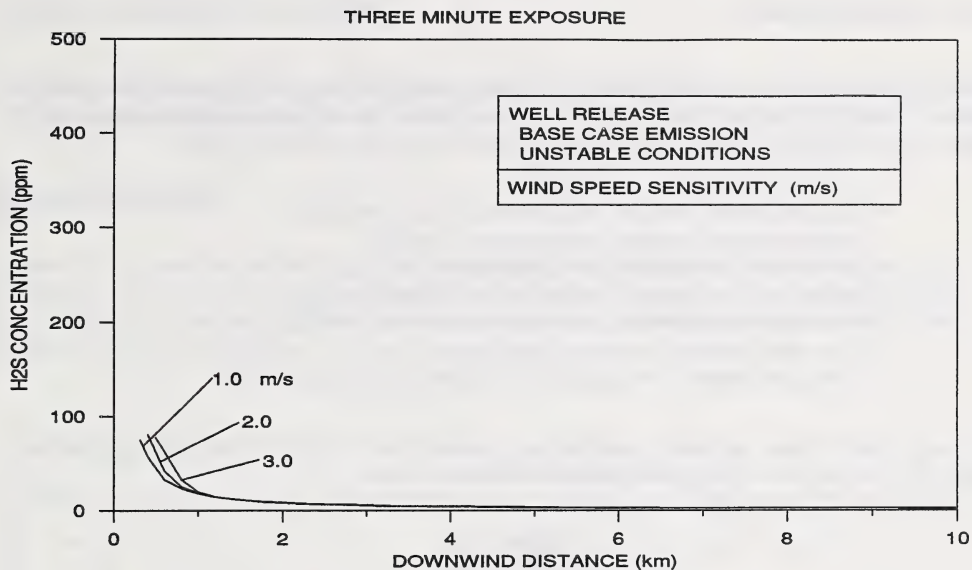


Figure 5.20

Predicted H₂S Concentrations for Selected Wind Speeds (Unstable Conditions).

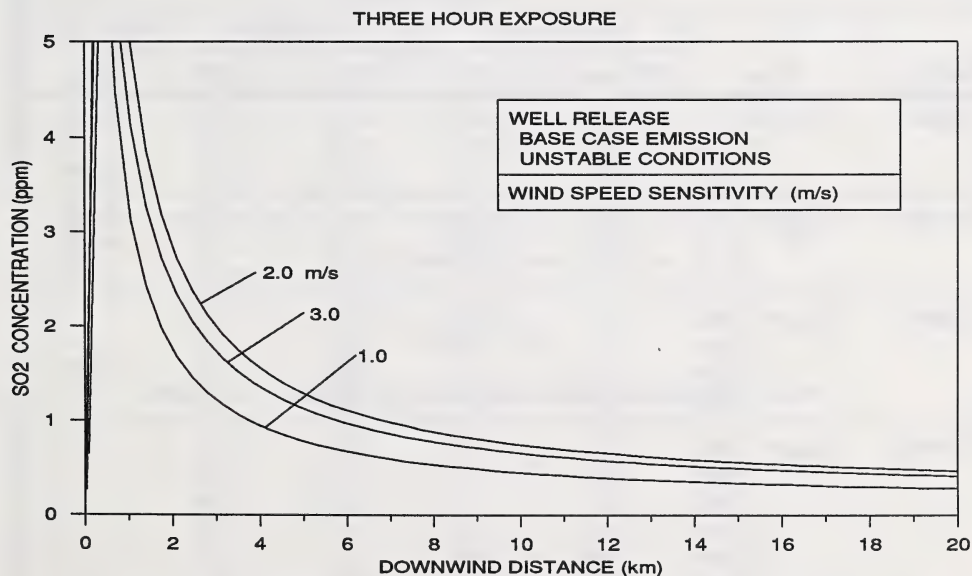


Figure 5.21

Predicted SO₂ Concentrations for Selected Wind Speeds (Unstable Conditions).

5.3.2 Hazard Zones

Distances to critical concentration values (hazard zones) are interpolated from the downwind distance concentration profiles. Table 5.21 summarizes the hazard zones associated with meteorology sensitivity runs. The largest hazard zones are associated with:

- Small values of surface roughness (for H₂S and SO₂)
- Large values of ambient temperature (for H₂S)
- Low wind speeds for stable conditions (for H₂S)
- Moderate wind speeds for stable conditions (for SO₂)
- Moderate wind speeds for neutral conditions (for H₂S)
- High wind speeds for neutral conditions (for SO₂)
- Low wind speeds for unstable conditions (for H₂S and SO₂)

For large travel times, the same cautions as presented for Table 5.11 are also applicable, especially for the low wind speed stable conditions.

Table 5.21

**Hazard Zone Sensitivity to Meteorological Parameters
(Base Case Well Blowout).**

		Distance (km) to:				
Stability	Case	3 minute H ₂ S		1 hour H ₂ S		3 hour SO ₂
		100 ppm	20 ppm	5 ppm	1 ppm	1 ppm
Stable	$Z_o = 0.1$ m	3.7	> 10	> 10	> 10	> 20
	0.3 m	2.8	> 10	> 10	> 10	0
	1.0 m	1.5	5.3	> 10	> 10	N/A
Stable	$T_{Ao} = 20$ °C	5.2	> 10	> 10	> 10	> 20
	0 °C	3.7	> 10	> 10	> 10	> 20
	-20 °C	3.7	> 10	> 10	> 10	> 20
Stable	$U_{REF} = 1$ m/s	3.7	> 10	> 10	> 10	0
	2 m/s	1.9	6.2	> 10	> 10	0
	3 m/s	1.2	2.9	5.0	> 10	> 20
	5 m/s	0.9	1.7	2.6	7.5	0
Neutral	$U_{REF} = 1$ m/s	0.3	0.4	0.5	8.3	0
	2 m/s	0.3	1.7	3.2	> 10	0
	3 m/s	0.7	1.8	2.9	9.4	0
	5 m/s	0.6	1.5	2.4	7.3	0
	10 m/s	0.4	0.8	1.1	2.7	0
	15 m/s	0.3	0.6	0.9	2.1	1.9
Unstable	$U_{REF} = 1$ m/s	0.3	0.9	1.9	> 10	3.8
	2 m/s	0.4	1.0	1.9	> 10	6.8
	3 m/s	0.5	1.0	1.8	9.6	5.8

5.3.3 Probability of Lethality

For the base case well blowout release scenario, sensitivity tests were done for the meteorological parameters given in Table 5.14.

Surface Roughness

Figure 5.22 shows the probability of lethality under the plume centreline versus downwind distance for this sensitivity test. Generally, the smaller the surface roughness, the higher the probability of lethality. This is because dispersion is enhanced near the surface for large values of surface roughness.

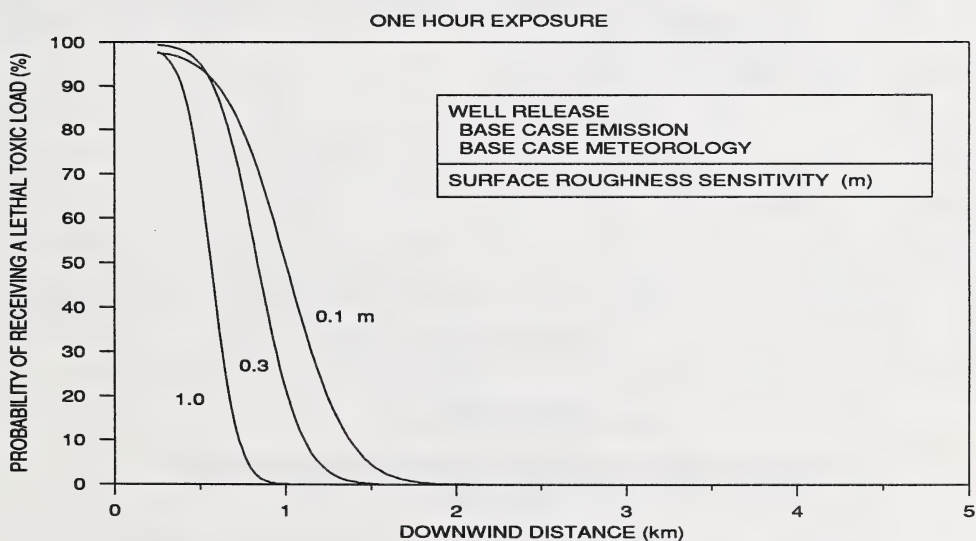


Figure 5.22

Predicted Lethality for Selected Surface Roughness Values.

Ambient Temperature

A sensitivity analysis was undertaken for three ambient temperature values, using the base case meteorology for all other parameters. Figure 5.23 shows the lethality curves. Higher ambient temperatures are associated with larger probabilities of fatality as plume rise is less.

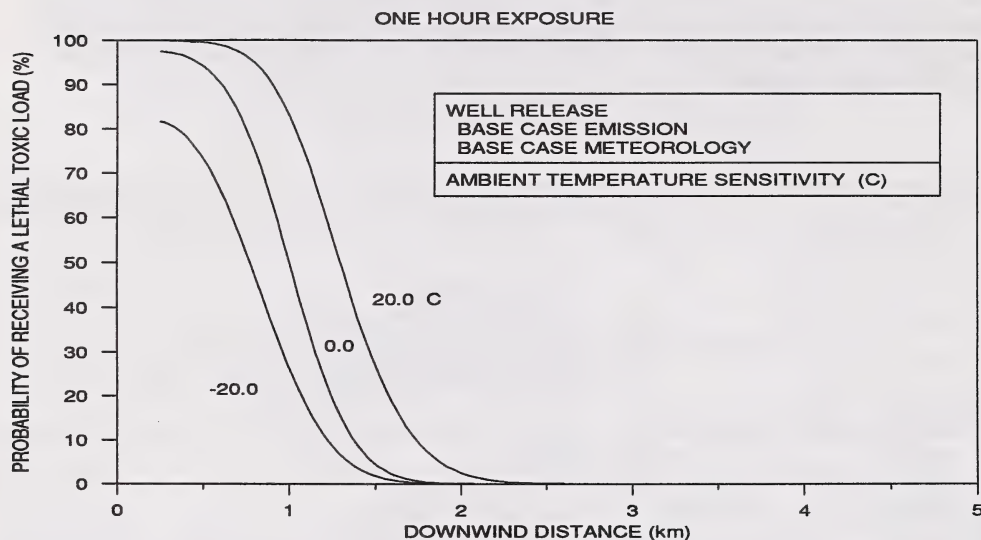


Figure 5.23

Predicted Lethality for Selected Ambient Temperatures.

Stable Conditions

Four wind speeds were examined for stable conditions, with the base case emission and (otherwise) base case meteorology. Figure 5.24 shows the lethality curves for the different wind speeds. The largest probabilities occur for the smallest wind speed of 1 m/s. The major effect of wind speed is an increase in downwind H_2S concentration due to decreasing along-wind dilution with decreasing wind speed. A secondary competing effect is the increasing plume height with decreasing wind speed.

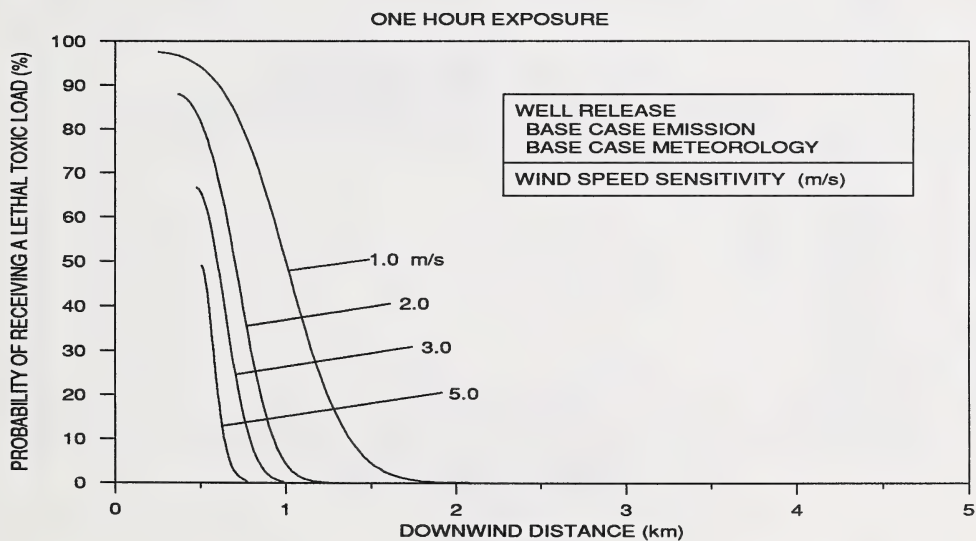


Figure 5.24

Predicted Lethality for Selected Wind Speeds (Stable Conditions).

Neutral Conditions

Six wind speed values were examined in neutral conditions. Figure 5.25 shows the lethality curves for the base case emission. The maximum probability of lethality occurs for a wind speed of 5 m/s, although the downwind extent of probability of lethality greater than zero is only 500 m (compared to 2 km for stable).

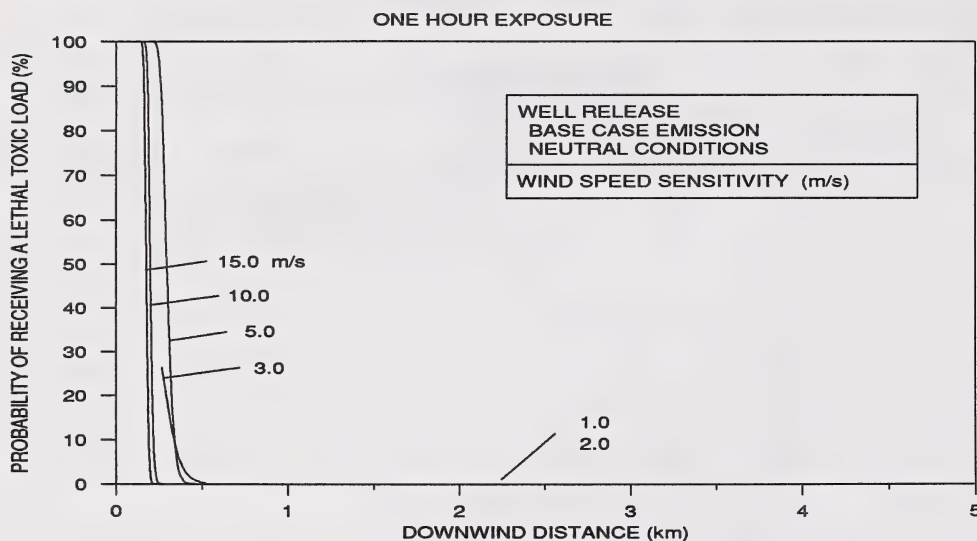


Figure 5.25

Predicted Lethality for Selected Wind Speeds (Neutral Conditions).

Unstable Conditions

Three wind speed values were examined for unstable conditions with base case well emission. Figure 5.26 shows that the predicted lethality for the three wind speeds is zero as the high plume rise and dispersion dilutes the concentrations. Actually, a decrease in lethality from 100% to 0% occurs within several hundred metres of the well but is not shown on the model output.

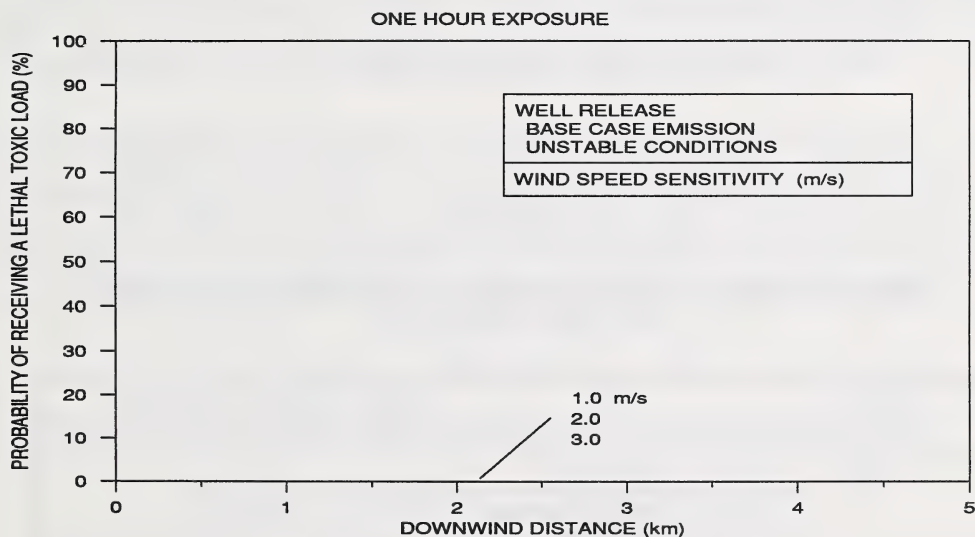


Figure 5.26

Predicted Lethality for Selected Wind Speeds (Unstable Conditions).

5.3.4 Potential Fatalities

Table 5.22 summarizes the potential number of fatalities associated with the meteorology sensitivity runs.

The largest potential number of fatalities are associated with:

- Small values of surface roughness
- Large value of ambient temperature
- Low wind speeds for stable conditions
- Moderate to high wind speeds for neutral conditions

Table 5.22

**Potential Number of Fatalities Sensitivity to Meteorological Parameters
(Base Case Well Blowout).**

Stability	Case	Potential Number of Fatalities
Stable	$Z_0 = 0.1 \text{ m}$	5
	$Z_0 = 0.3 \text{ m}$	3
	$Z_0 = 1.0 \text{ m}$	2
Stable	$T_A = -20 \text{ }^\circ\text{C}$	3
	$T_A = 0.0 \text{ }^\circ\text{C}$	5
	$T_A = +20 \text{ }^\circ\text{C}$	6
Stable	$U_{REF} = 1 \text{ m/s}$	5
	$U_{REF} = 2 \text{ m/s}$	2
	$U_{REF} = 3 \text{ m/s}$	1
	$U_{REF} = 5 \text{ m/s}$	0.4
Neutral	$U_{REF} = 1 \text{ m/s}$	0
	$U_{REF} = 2 \text{ m/s}$	0
	$U_{REF} = 3 \text{ m/s}$	0
	$U_{REF} = 5 \text{ m/s}$	0.4
	$U_{REF} = 10 \text{ m/s}$	0.2
	$U_{REF} = 15 \text{ m/s}$	0.1
Unstable	$U_{REF} = 1 \text{ m/s}$	0
	$U_{REF} = 2 \text{ m/s}$	0
	$U_{REF} = 3 \text{ m/s}$	0

5.4 Pipeline Rupture Source Parameters

Pipeline rupture location, pipeline size, geometries, release angle, excess mass by ESD valves and hole size were varied to observe the effect on predictions. Note that 3 minute average H_2S concentrations are presented in all of the following discussion.

Exposure Time

For a pipeline rupture where all the ESD valves close, the releases are transient and the duration of the sour gas cloud at any given point downwind depends on the duration of the release, the wind speed and the along wind plume dilution. Figure 5.27 shows the transient H_2S concentration-time profile for the base case pipeline emission (Table 5.4) and meteorology (Table 5.6) release scenario at selected downwind distances.

The time the selected H_2S concentration criteria are exceeded is given in Table 5.23. The 100 and 20 ppm H_2S concentration criteria refer to peak concentration values based on three-minute average values of σ_y . For wind speed values larger than the base case value of 1 m/s, the predicted peaks for the downwind distances shown in the figure will occur sooner after the rupture and will be of a shorter duration. Predicted peak H_2S concentrations are relatively large but of relatively short duration. Under these circumstances, indoor H_2S concentrations are expected to be much less than the outdoor values (Wilson, 1986).

Table 5.23

Duration of Time Predicted H_2S Concentration Exceeds the Indicated Values.

Duration (min) that concentration exceeds indicated value.		
Distance (km)	100 ppm	20 ppm
1	4	6
2	5	10
5	0*	15
10	0*	0*

* Maximum H_2S concentration less than indicated value.

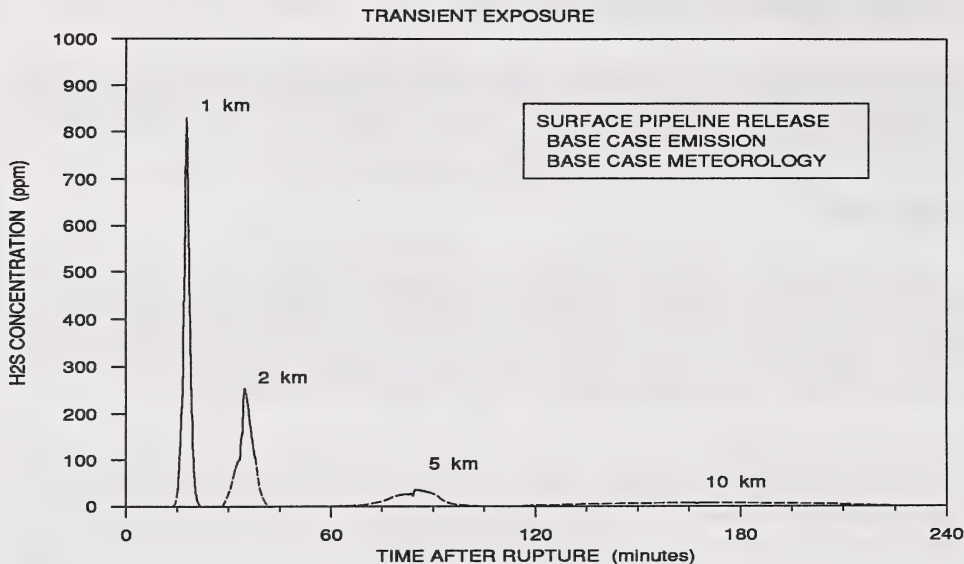


Figure 5.27

Predicted H₂S Concentrations from a Pipeline Rupture as a Function of Time.

5.4.1 Concentration Profiles

Rupture Location

Sensitivity analyses were undertaken for the four pipeline rupture scenarios shown in Table 5.24. All of the releases were modelled as an above ground ($Z_E = 1.0$), horizontal jet ($C_D = 0$).

Figure 5.28 shows the mass release rate for the selected rupture scenarios. The initial release rate depends on the number of pipeline segments which deplete. That is, two independent segments (Rupture Scenarios 2 and 3) result in twice the initial mass release rate than a single segment (Rupture Scenarios 1 and 4). Shorter lengths of pipeline (Rupture Scenario 3) deplete faster than the longer lengths (Rupture Scenarios 1, 2 and 4).

For Rupture Scenario 4, a steady-state release rate of $240 \cdot 10^3 \text{ m}^3/\text{d}$ (3.0 kg/s) was assumed. This value is much less than the peak transient release value (at time = 0) and does not dominate the transient release value until about 59 s. Until this time, the release rate is identical to that given for Rupture Scenario 1. For this reason, Rupture Scenario 4 was not shown in Figure 5.28.

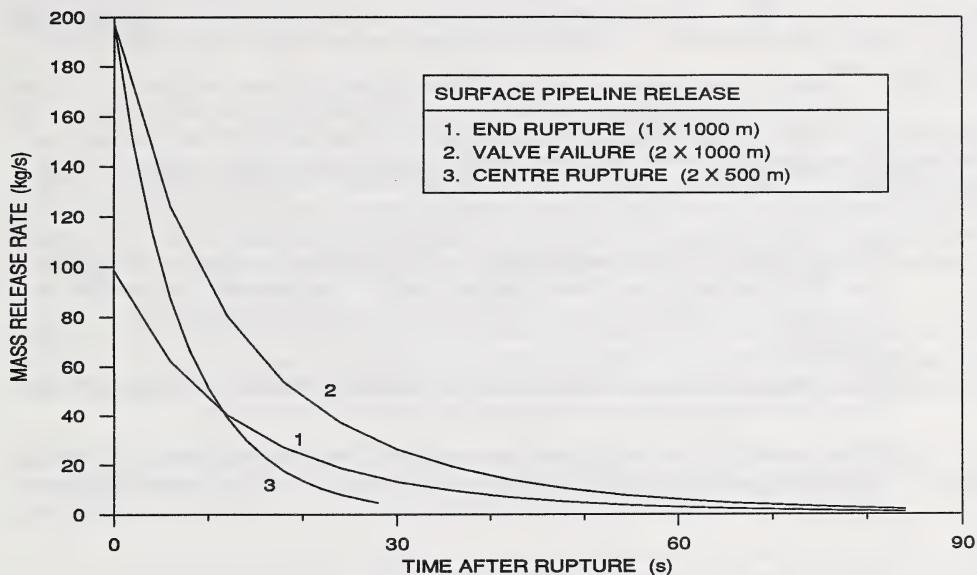


Figure 5.28

Predicted Mass Release Rate for Selected Pipeline Rupture Flow Scenarios.

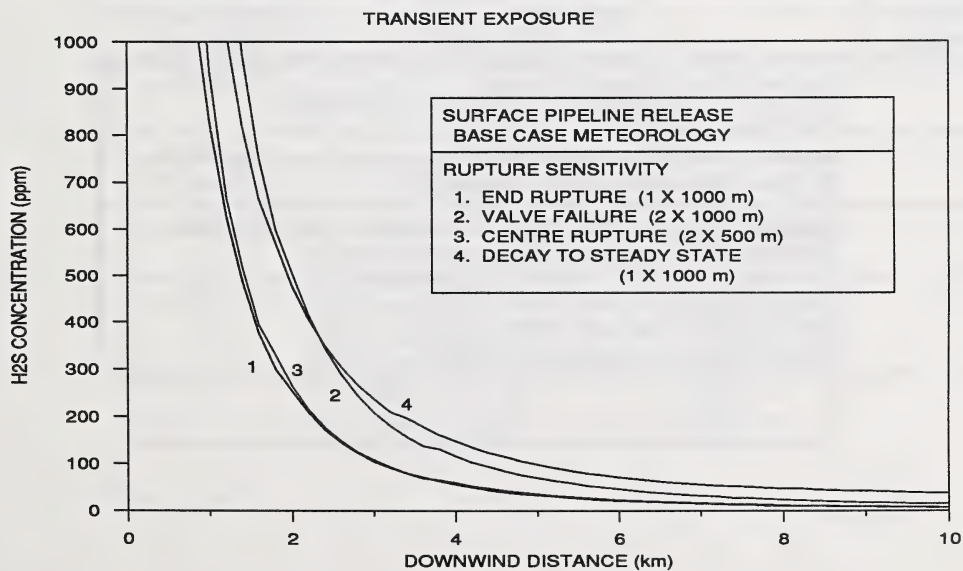


Figure 5.29

Predicted Peak H₂S Concentrations for Selected Pipeline Rupture Flow Scenarios.

The times to deplete 99% of the pipeline contents are 94 s for Rupture Scenarios 1 and 2 and 35 s for Rupture Scenario 3. The depletion time is proportional to the length of the pipeline segment.

Figure 5.29 shows the predicted H_2S concentration as a function of downwind distance and the selected flow scenarios. From the figure and the associated computer output it can be noted that:

- The predicted H_2S concentration profile is not sensitive to where in the pipeline the break occurs for a given pipeline length. For example, the profile for Scenario 1 (1 x 1000 m segment) is similar to that for Scenario 3 (2 x 500 m segments).
- The predicted H_2S concentrations for two lengths (Scenario 2) are about double those for a pipeline segment one-half the length (Scenario 1).
- The transient release which decays to a steady state value (Scenario 4) results in larger predicted H_2S concentration than for the purely transient release (Scenario 1) at the larger downwind distances.

Table 5.24

Surface Pipeline Rupture Location Sensitivity Assumptions.

Rupture Scenario	Description	Pipeline Length Depleted
1	Rupture adjacent to an ESD valve. All ESD valves operate as designed.	1 x 1000 m
2	Rupture at an ESD valve which fails. All other ESD valves operate as designed.	2 x 1000 m
3	Rupture halfway between two ESD valves. All ESD valves operate as designed.	2 x 500 m
4	Rupture in segment next to well head. Well ESD valve fails, all others operate. Transient decay to steady-state release.	1 x 1000 m

Pipeline Size

Sensitivity analyses were undertaken for the four pipeline diameters shown in Table 5.25. Two lengths were considered for a 10 inch diameter pipeline, 1000 and 3000 m.

Figure 5.30 shows the mass release rate for the selected size scenarios. The initial release rate depends on the pipeline diameter (or more exactly the diameter of the release opening which in this case is assumed to be identically equal to the internal diameter of the pipeline). The longer the pipeline, the longer for the pipeline to vent its contents to the atmosphere.

The times to deplete 99% of the pipeline contents for the 4, 6, 8 and 10 inch 1000 m lines are 16, 94, 82 and 74 seconds respectively. Increasing the length to 3000 m increases the depletion time for the 10, 14 and 16 inch lines to 383, 334 and 310 seconds respectively.

Figure 5.31 shows the predicted H₂S concentration as a function of downwind distance and the selected size scenarios. From the figure and the associated computer output it can be noted that:

- The predicted H₂S concentration profile is sensitive to the pipeline diameter. The larger the diameter, the larger the predicted H₂S concentration values.
- The predicted H₂S concentrations for Scenario 4 (3000 m pipeline, 10 inch) are higher than for Scenario 5 (1000 m pipeline, 10 inch).

Table 5.25

Pipeline Size Sensitivity Assumptions.

Scenario	Diameter	Pipeline Length Depleted
1	154.1 mm (6 inch)	1 x 1000 m
2	102.3 mm (4 inch)	1 x 1000 m
3	202.7 mm (8 inch)	1 x 1000 m
4	254.5 mm (10 inch)	1 x 1000 m
5	254.5 mm (10 inch)	1 x 3000 m
6	330.2 mm (14 inch)	1 x 3000 m
7	381.0 mm (16 inch)	1 x 3000 m

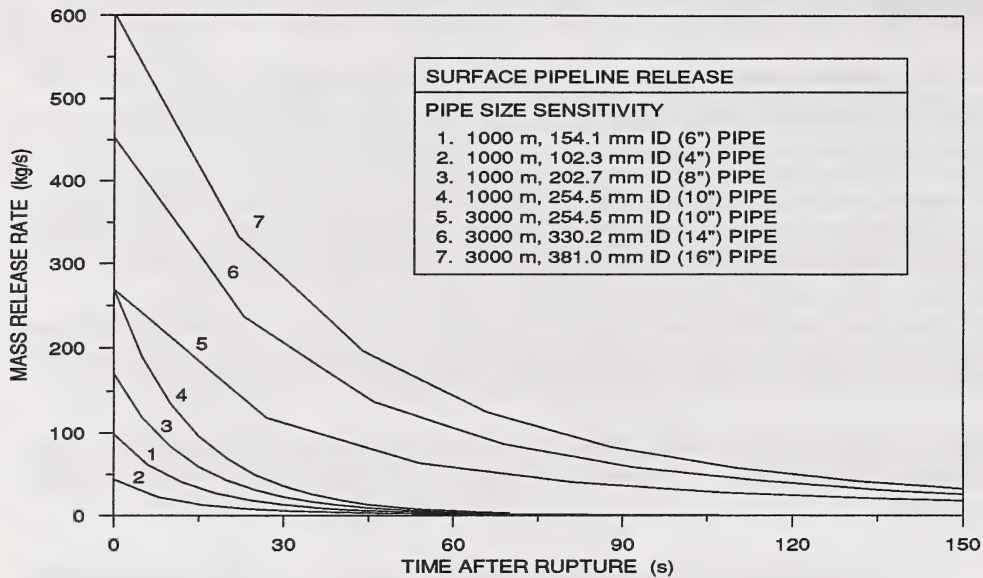


Figure 5.30

Predicted Mass Release Rate for Selected Pipeline Size Scenarios.

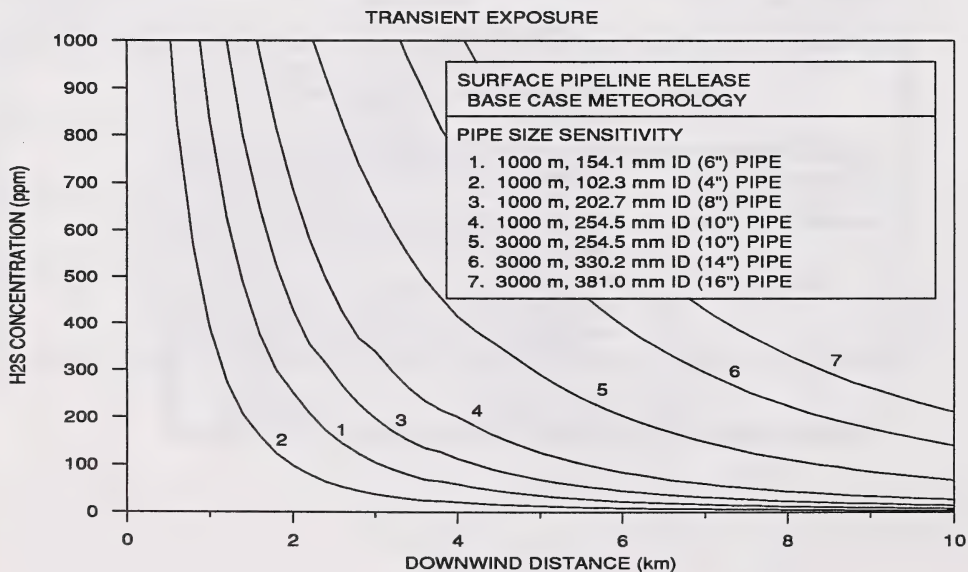


Figure 5.31

Predicted Peak H₂S Concentrations for Selected Pipeline Size Scenarios.

Buried Pipe Emission Angle

Sensitivity analysis were undertaken for a buried, 3000 m long, 254.5 mm (10 inch) internal diameter pipeline (Scenario 5 of pipeline size sensitivity tests). The effect of drag on the jet due to the crater walls was accounted for by setting $C_D = 2.0$. The release angle out of the crater was varied assuming an end release, near the ESD valve with the exit height set at ground level ($Z_E = 0.0$).

Figure 5.32 shows the predicted H_2S concentration as a function of distance for the selected emission angles. The following observations can be made:

- Higher downwind concentrations result when drag due to the crater and a ground level release are assumed. The 0° curve of Figure 5.32 is higher than the Scenario 5 curve of Figure 5.31 starting at about 2 km downwind.
- Near the pipeline, the predicted H_2S concentration is very sensitive to the emission angle. Concentrations decrease from a maximum for the 0° release to near zero for the 45° release.
- Far downwind (~ 7 km), the predicted concentration is independent of the release angle.

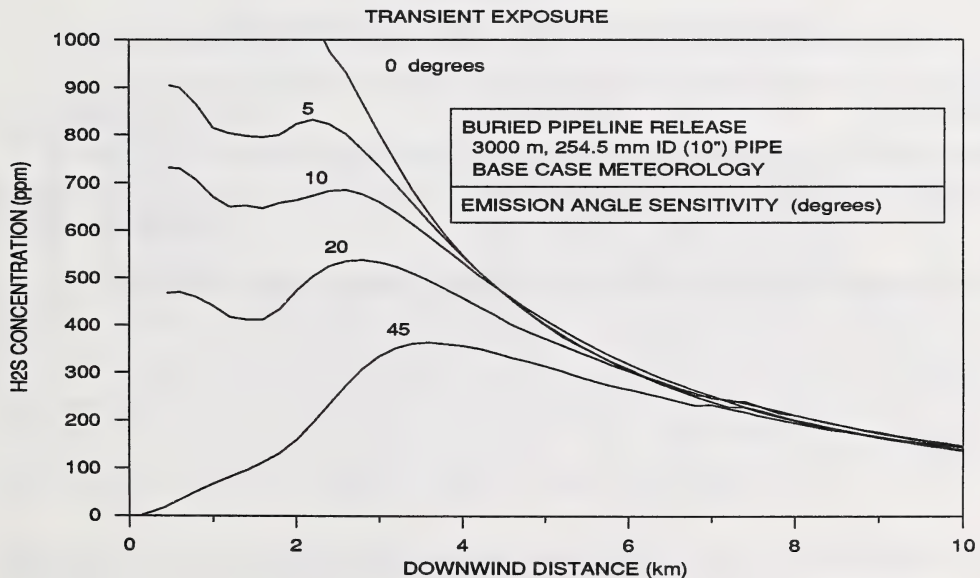


Figure 5.32

Predicted Peak H_2S Concentrations for Selected Emission Angles from Buried Pipeline.

Geometry

Sensitivity analyses were undertaken for the selected pipeline rupture geometries shown in Table 5.26.

Figure 5.33 shows the predicted H₂S concentration as a function of downwind distance for the selected release geometries. From the figure and the associated computer output it can be noted that:

- Horizontal jet releases (Scenarios 1 and 3) result in larger predicted H₂S concentration values.
- Downwind jet releases (Scenario 1) results in greater predicted H₂S concentration values than upwind jet releases (Scenario 3).
- Vertical and cloud releases (Scenarios 2 and 4) result in smaller predicted H₂S concentration values, especially near the pipeline.
- Vertical releases (Scenario 2) results in the smallest predicted H₂S concentration values.

Table 5.26

Pipeline Rupture Geometry Sensitivity Assumptions.

Geometry	Description	Pipeline Length Depleted
1	Downwind Jet (Side rupture $\lambda = 0^\circ$).	1 x 1000 m
2	Vertical Jet (Top rupture $\lambda = 90^\circ$).	1 x 1000 m
3	Upwind Jet (Side rupture $\lambda = 180^\circ$).	1 x 1000 m
4	Cloud (Bottom rupture $\lambda = 0^\circ$, $C_D = 3$).	1 x 1000 m

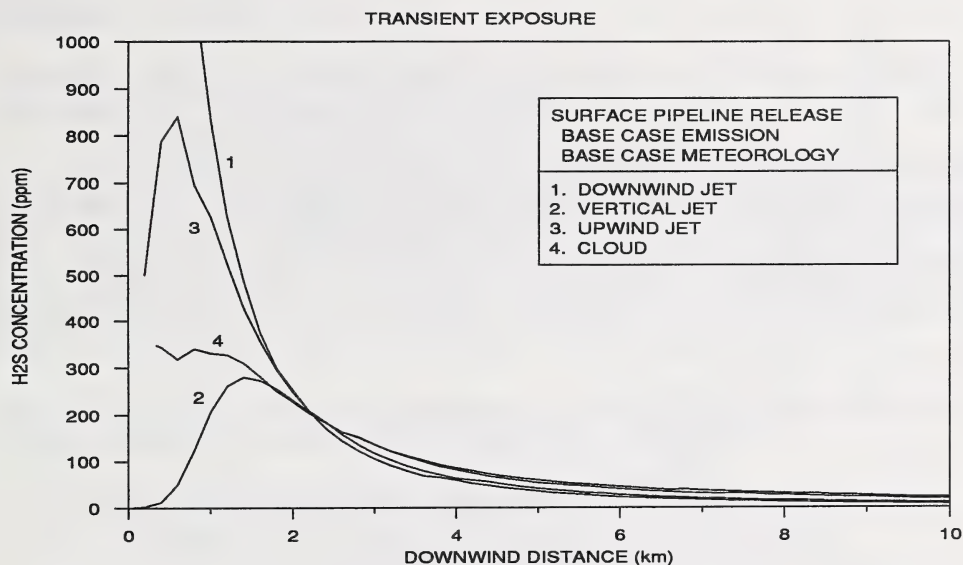


Figure 5.33

Predicted Peak H₂S Concentrations for Selected Pipeline Rupture Geometries.

Excess Mass

Sensitivity analyses were undertaken for 10, 30, 100 and 200% excess mass scenarios for the base case pipeline.

Figure 5.34 shows the mass release rate for the selected excess mass scenarios. For all cases, the initial release rates are the same. The larger the excess mass, the longer the time to depressure the pipeline. The times to deplete 99% of the pipeline contents are 95, 94, 105 and 211 s for the 10, 30, 100 and 200% excess mass scenarios, respectively. The model predicts a slightly shorter time to evacuate more mass for the 30% case than for the 10% case as the flow rate is higher. This is a limitation of the double exponential blowdown release rate approach and does not affect final results. One would expect the release rate to be independent of the excess mass factor until the ESD valves begin to close.

Figure 5.35 shows the predicted H₂S concentration as a function of downwind distance for the selected excess mass scenarios. From the figure it can be noted that:

- The predicted H₂S concentration profile is sensitive to the delay time for the ESD valves to fully isolate the ruptured pipeline segment from the rest of the gas gathering system (excess mass).
- The effect of increasing the excess mass from 10 to 200% has the effect of more than doubling the H₂S concentration.

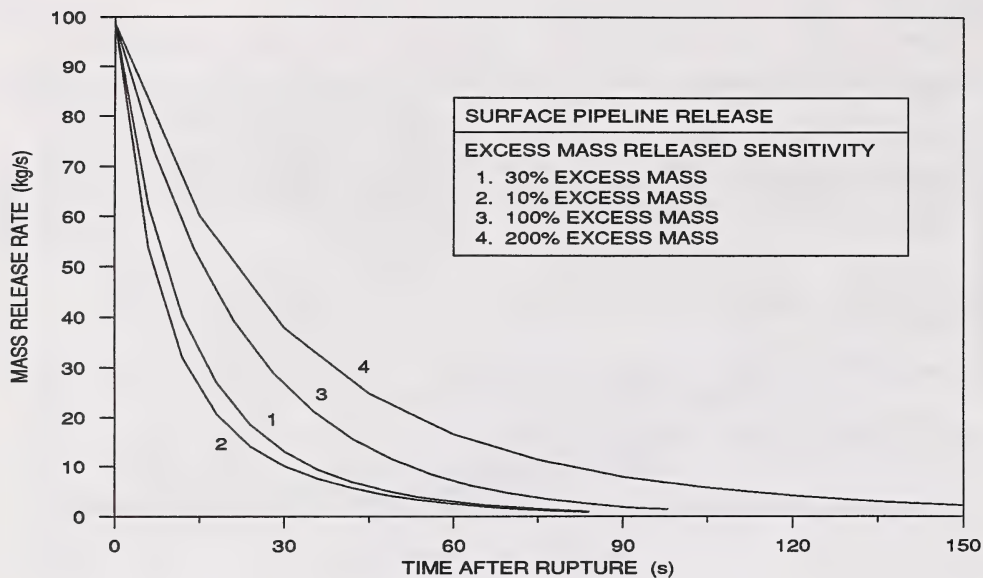


Figure 5.34

Predicted Mass Release Rate for Selected Excess Mass Scenarios.

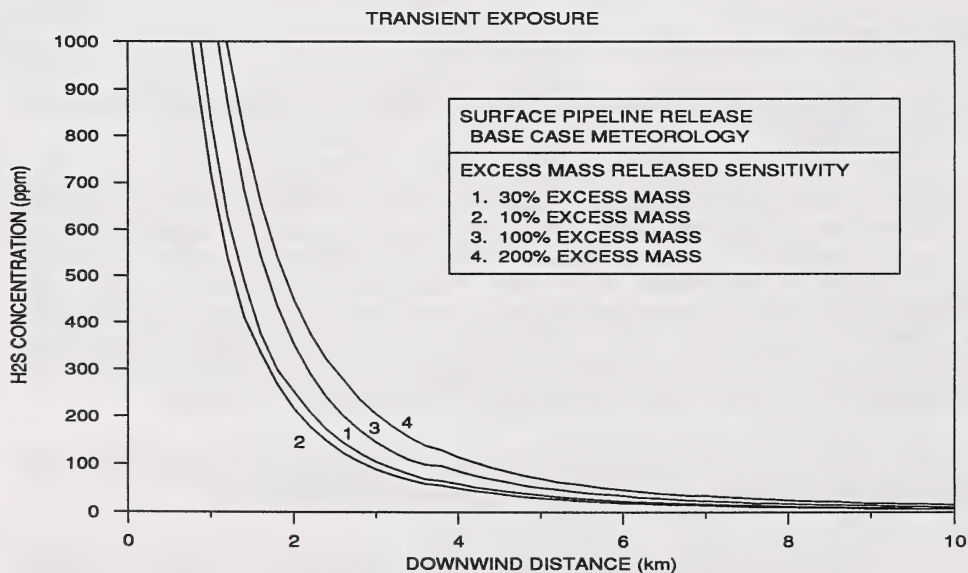


Figure 5.35

Predicted Peak H₂S Concentrations for Selected Excess Mass Scenarios.

Hole Size

Sensitivity analyses were undertaken for hole sizes of 100, 50, 25, 10 and 5% in the base case pipeline.

Figure 5.36 shows the mass release rate for the selected hole sizes. The initial rate increases with the hole size. The time to depressure the pipeline increases substantially for smaller hole sizes. The time to deplete 99% of the pipeline contents are 94, 147, 477, 1655 and 3552 s for the 100, 50, 25, 10 and 5% hole size scenarios, respectively. Note that the same amount of mass is released in each case as the excess mass has been held constant at 30% and the excess mass will probably increase for smaller hole sizes as the ESD valves take longer to activate (or in the extreme, may not activate for the smaller hole sizes).

Figure 5.37 shows the predicted H₂S concentration as a function of downwind distance for the selected hole size scenarios. From the figures, it can be noted that:

- The maximum H₂S concentrations occur for a full rupture (100% hole).
- Predicted downwind H₂S concentrations decrease with hole size.
- Peak concentrations of the large holes (100 and 50%) are due to the later portion of the release while for the small holes (25, 10 and 5%), peak concentrations are due to the initial portion of the release.

5.4.2 Hazard Zones

Table 5.27 summarizes the hazard zones associated with the pipeline rupture sensitivity runs. Only the 3 minute average concentration criteria are presented as the releases do not last one hour.

Values expressed as an inequality either exceed the distance or the time limits specified by the model. At large downwind distances, the effects due to different release geometries become negligible. The largest hazard zones are associated with horizontally directed releases, large pipeline diameters, long pipeline lengths or buried pipes. Note that for large travel times, the same cautions presented for steady releases are applicable.

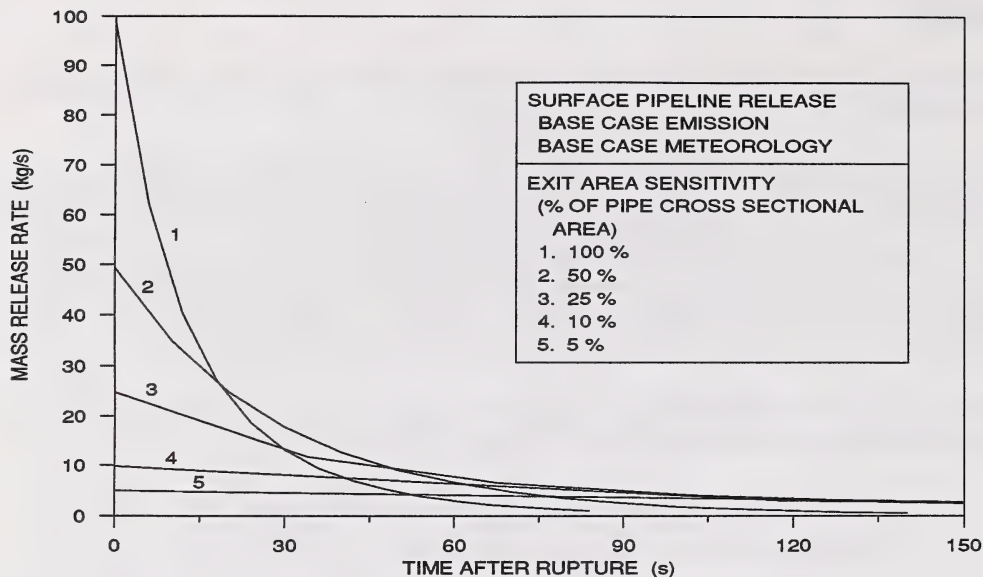


Figure 5.36

Predicted Mass Release Rate for Selected Hole Size Scenarios.

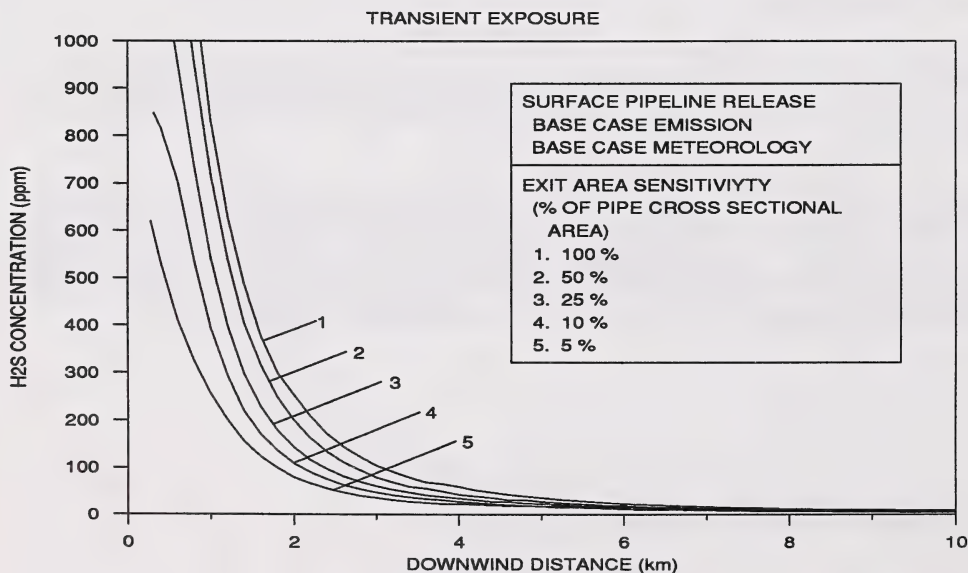


Figure 5.37

Predicted Peak H₂S concentrations for Selected Hole Size Scenarios.

Table 5.27

**Hazard Zone Sensitivity to Pipeline Rupture Parameters
(Base Case Meteorology).**

		Distance (km) to:	
Case	Description	Transient H ₂ S	
		100 ppm	20 ppm
Rupture 1	1 x 1000 m	3.1	6.3
Rupture 2	2 x 1000 m	4.3	8.5
Rupture 3	2 x 500 m	3.1	6.1
Rupture 4	1 x 1000 m decay to steady state	4.9	> 10
Size 1	6 inch (1 x 1000 m)	3.1	4.6
Size 2	4 inch (1 x 1000 m)	2.0	3.3
Size 3	8 inch (1 x 1000 m)	4.2	5.8
Size 4	10 inch (1 x 1000 m)	5.5	6.6
Size 5	10 inch (1 x 3000 m)	8.3	> 10
Size 6	14 inch (1 x 3000 m)	> 10	> 10
Size 7	16 inch (1 x 3000 m)	> 10	> 10
Buried Pipe 1	0°	> 10	> 10
Buried Pipe 2	5°	> 10	> 10
Buried Pipe 3	10°	> 10	> 10
Buried Pipe 4	20°	> 10	> 10
Buried Pipe 5	45°	> 10	> 10
Geometry 1	Downwind Jet	3.1	6.3
Geometry 2	Vertical Jet	3.6	> 10
Geometry 3	Upwind Jet	3.2	6.9
Geometry 4	Cloud	3.6	9.4
Excess Mass 1	10%	2.9	5.9
Excess Mass 2	30%	3.1	6.3
Excess Mass 3	100%	3.6	7.5
Excess Mass 4	200%	4.3	8.8
Hole Size 1	100%	3.1	6.3
Hole Size 2	50%	2.8	5.7
Hole Size 3	25%	2.4	5.3
Hole Size 4	10%	2.1	4.6
Hole Size 5	5%	1.8	4.3

5.4.3 Probability of Lethality

Flow Rate

Table 5.24 shows the four pipeline rupture scenarios considered in this sensitivity test. Figure 5.38 shows the lethality curves for the four rupture scenarios. The sour gas release rate depends on the number of pipeline segments which deplete. Two independent segments (Scenario 2 and 3) have twice the initial mass rate of single segments (Scenarios 1 and 4). Shorter lengths (Scenario 3) deplete faster than longer lengths (Scenarios 1, 2 and 4).

From Figure 5.38 it can be seen that:

- The lethality curves are not sensitive to where the rupture occurs in the pipeline. Scenario 1 (1 x 1000 m segment) results in a similar lethality curve to Scenario 3 (2 x 500 m segments).
- The transient release which decays to a steady rate (Scenario 4) results in larger probabilities of lethality than the purely transient release (Scenario 1).
- The highest probability of lethality result from rupture Scenario 2.

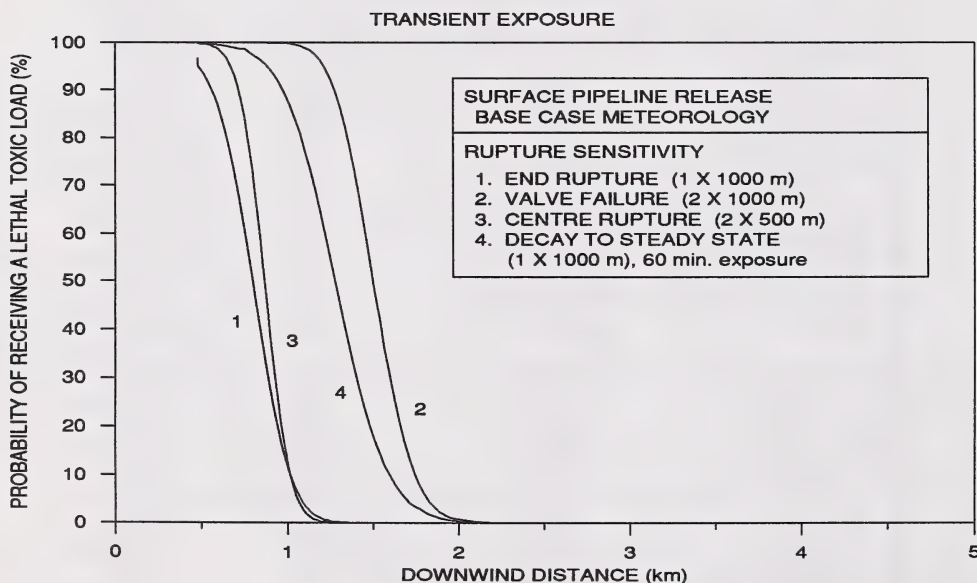


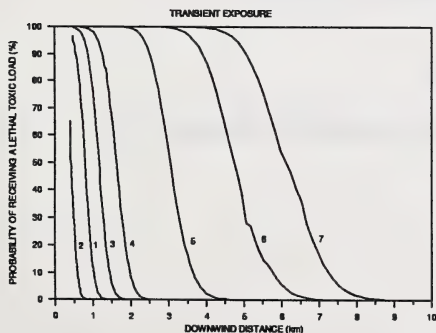
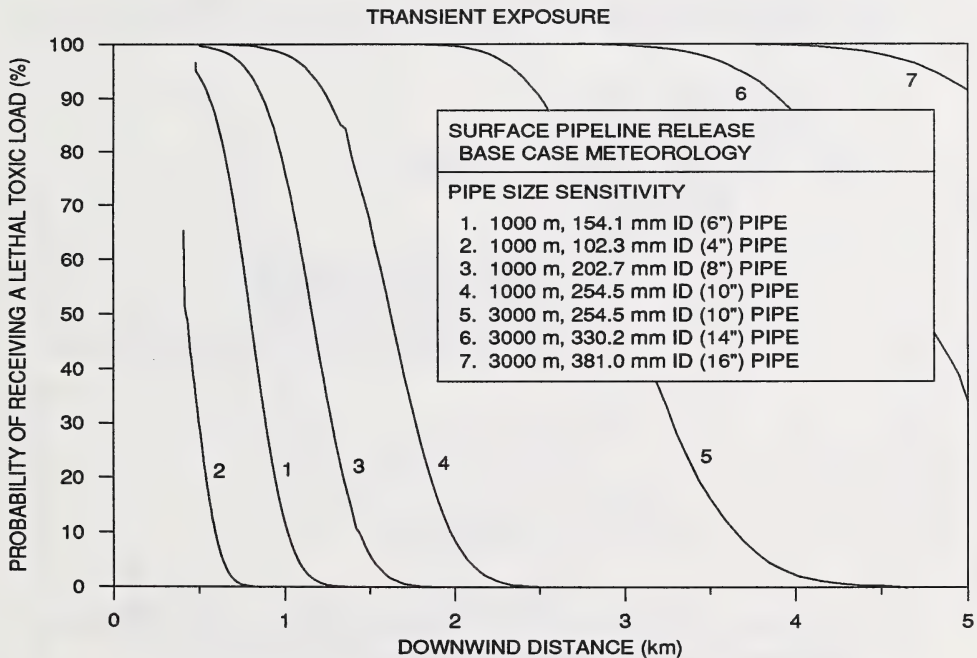
Figure 5.38

Predicted Lethality for Selected Pipeline Rupture Flow Scenarios.

Pipeline Size

A sensitivity analysis was undertaken for seven pipeline diameters as shown in Table 5.27. Figure 5.39 shows the lethality curves for these pipeline size scenarios. From the figure one observes that:

- The larger the pipeline diameter, the higher the probability of lethality.
- Increasing the pipeline length increases the probability of lethality (Scenario 4 and 5).



Expanded Distance Scale.

Figure 5.39
**Predicted Lethality for
Selected Pipeline Size Scenarios.**

Buried Pipe Emission Angle

Figure 5.40 shows the effect the angle of release has on the predicted lethality profiles for a relatively large (3000 m long, 254.5 mm ID) buried pipe (Scenario 5 from Figure 5.39). The following is noted:

- The effect of the crater drag is to reduce the downwind lethality compared to the jet case (Scenario 5, Figure 5.39).
- Predicted lethality is very sensitive to release angle, approaching zero for a release angle of 20°.
- For a typical release angle of 45°, there is essentially no probability of lethality for this release scenario.

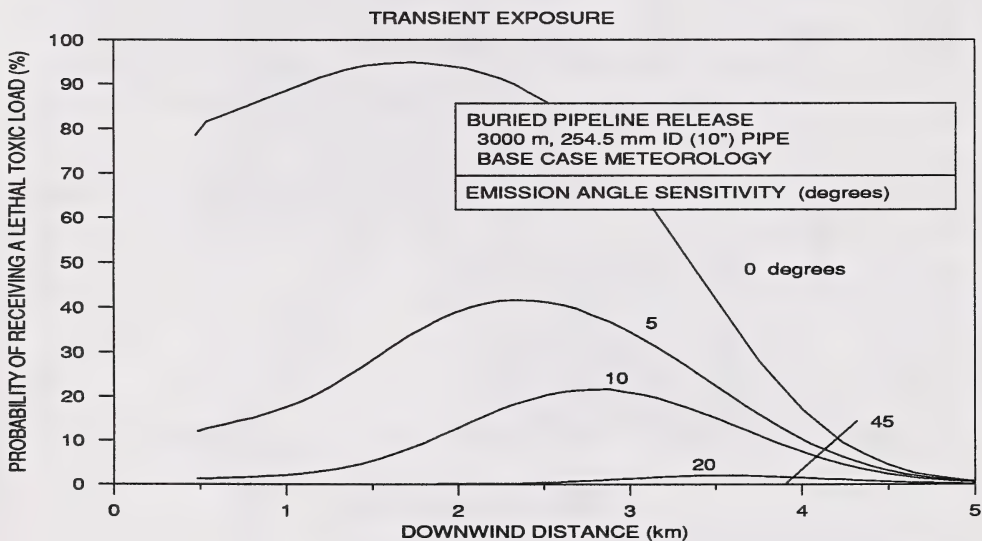


Figure 5.40

Predicted Lethality for Selected Emission Angles from Buried Pipe.

Geometry

Table 5.26 shows four pipeline rupture geometries used in this sensitivity test. Figure 5.41 shows the lethality curves for these geometries. From the figure it is evident that:

- Downwind jets (Scenario 1) result in the highest probabilities of lethality.
- Vertical jets, upwind jets and clouds result in no probability of lethality.

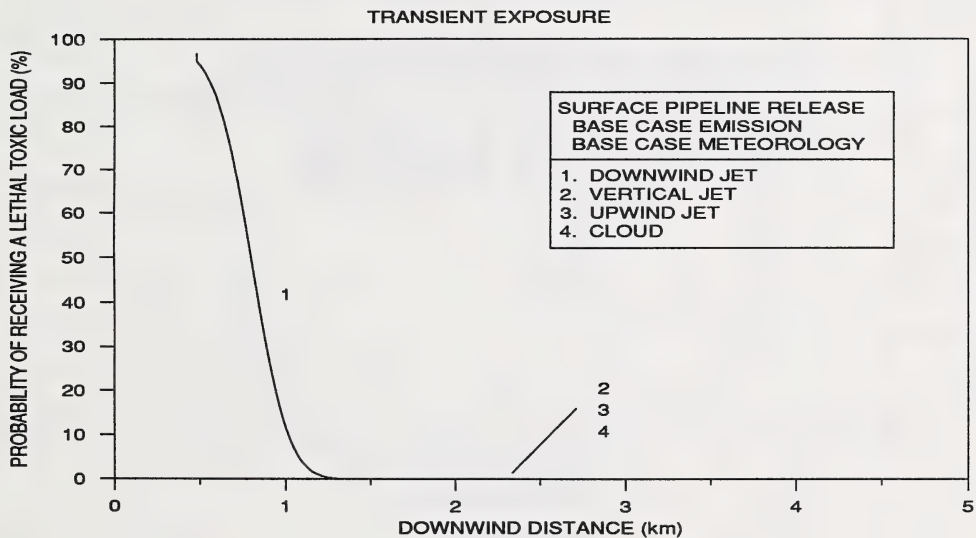


Figure 5.41

Predicted Lethality for Selected Pipeline Rupture Geometries.

Excess Mass

Figure 5.42 shows how the probability of lethality is sensitive to the excess mass. The more mass released, the higher the probability of lethality at a given downwind distance. The curves show the advantages of installing ESD valves which sense a rupture early and close quickly.

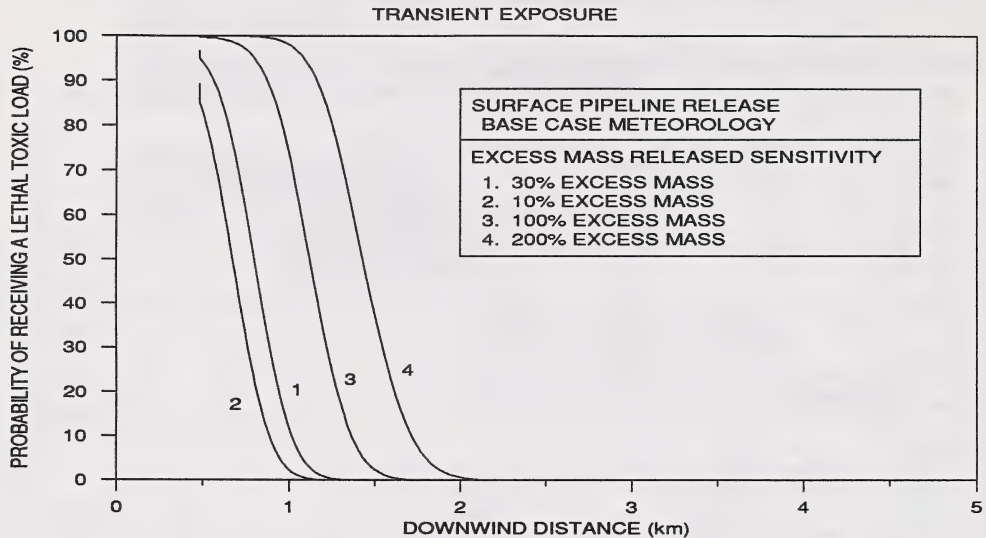


Figure 5.42

Predicted Lethality for Selected Excess Mass Scenarios.

Hole Size

Figure 5.43 shows the lethality curves for the various hole sizes modelled. Note that the maximum predicted lethality is not associated with the largest hole, although the maximum concentrations were associated with the largest hole size (Figure 5.37). This is because the duration of exposure is longer for the 50% hole than for the 100% hole. Small holes may be lethal up to 500 m downwind of the release.

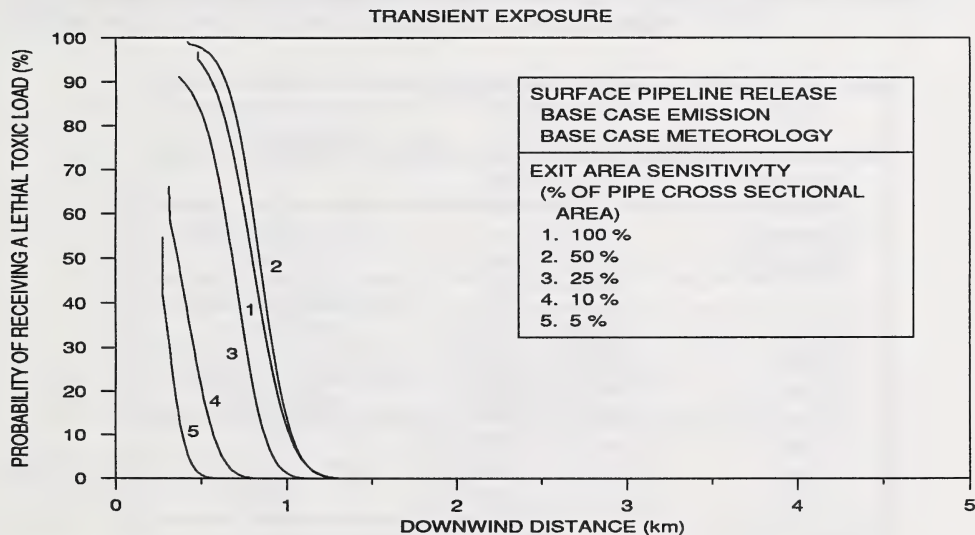


Figure 5.43
Predicted Lethality for Selected Hole Size Scenarios.

5.4.4 Potential Fatalities

The potential number of fatalities for the pipeline rupture sensitivity runs are summarized in Table 5.28. The largest potential number of fatalities are associated with horizontal releases, large pipeline diameters and long pipeline lengths, high excess mass and large hole sizes.

Table 5.28

**Potential Number of Fatalities Sensitivity to Pipeline Rupture Parameters
(Base Case Meteorology).**

Case	Description	Potential Number of Fatalities
Rupture 1	1 x 1000 m	2
Rupture 2	2 x 1000 m	7
Rupture 3	2 x 500 m	3
Rupture 4	1 x 1000 m decay to steady state	6
Size 1	6 inch (1 x 1000 m)	2
Size 2	4 inch (1 x 1000 m)	0.3
Size 3	8 inch (1 x 1000 m)	4
Size 4	10 inch (1 x 1000 m)	7
Size 5	10 inch (1 x 3000 m)	18
Size 6	14 inch (1 x 3000 m)	37
Size 7	16 inch (1 x 3000 m)	57
Buried Pipe 1	0°	11
Buried Pipe 2	5°	3
Buried Pipe 3	10°	1
Buried Pipe 4	20°	0.1
Buried Pipe 5	45°	0
Geometry 1	Downwind Jet	2
Geometry 2	Vertical Jet	0
Geometry 3	Upwind Jet	0
Geometry 4	Cloud	0
Excess Mass 1	10%	1
Excess Mass 2	30%	2
Excess Mass 3	100%	4
Excess Mass 4	200%	5
Hole Size 1	100%	2
Hole Size 2	50%	2
Hole Size 3	25%	1
Hole Size 4	10%	0.2
Hole Size 5	5%	0.1

5.5 Pipeline Rupture Meteorology Parameters

The base case meteorology used for the pipeline rupture evaluation is the same as that which was used for the well blowout sensitivity analysis. For the base case pipeline rupture release scenario, the sensitivity was evaluated for the selected meteorology parameters given in Table 5.29.

The same model default values for vertical temperature gradients of 0.03, -0.01 and -0.015 °C/m were assumed for stable, neutral and unstable conditions respectively. Similarly, unstable conditions assumed a mixing height (Z_i) of 100 m and a surface heat flux (H_o) of 50 W/m² and neutral conditions assumed a surface heat flux of -5 W/m².

Table 5.29
PBL Parameter Sensitivity Analysis.

Stable Conditions							
Wind Speed	U_{REF} (m/s)	1	2	3	5		
Neutral Conditions							
Wind Speed	U_{REF} (m/s)	1	2	3	5	10	15
Unstable Conditions							
Wind Speed	U_{REF} (m/s)	1	2	3	5		

5.5.1 Concentration Profiles

Stable Conditions

Figure 5.44 shows the predicted H₂S concentrations as a function of downwind distance and wind speed. The maximum H₂S concentrations occur with low wind speeds (~ 1 m/s).

Neutral Conditions

Figure 5.45 shows the predicted H₂S concentrations as a function of downwind distance and wind speed. The maximum H₂S concentration occurs with moderate wind speeds (~ 5 m/s).

Unstable Conditions

Figures 5.46 shows the predicted H₂S concentrations as a function of downwind distance and wind speed. The maximum H₂S concentration occurs with a wind speed of 3 m/s. As noted before, the model reclassifies the 5 m/s windspeed to neutral conditions.

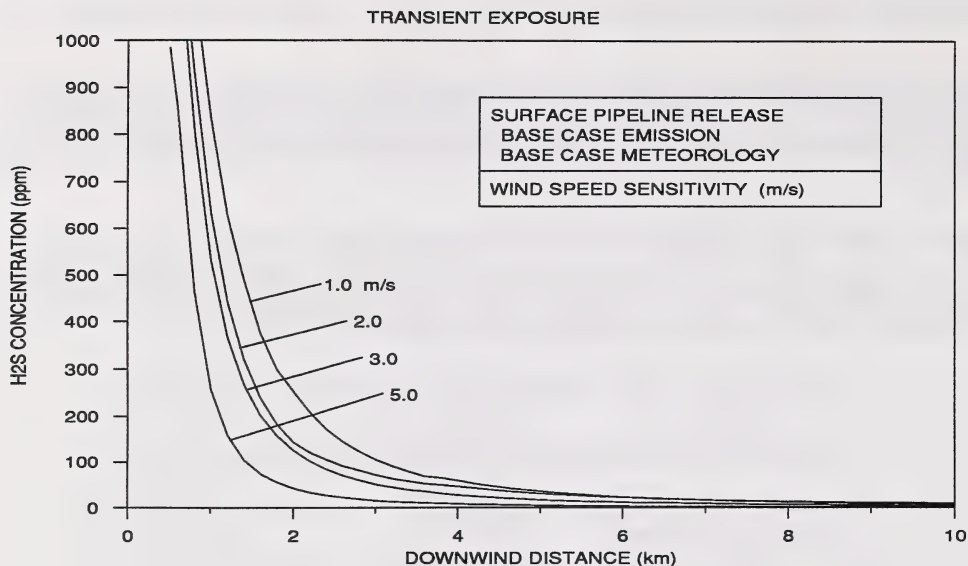


Figure 5.44

Predicted Peak H₂S Concentrations for Selected Wind Speeds (Stable Conditions).

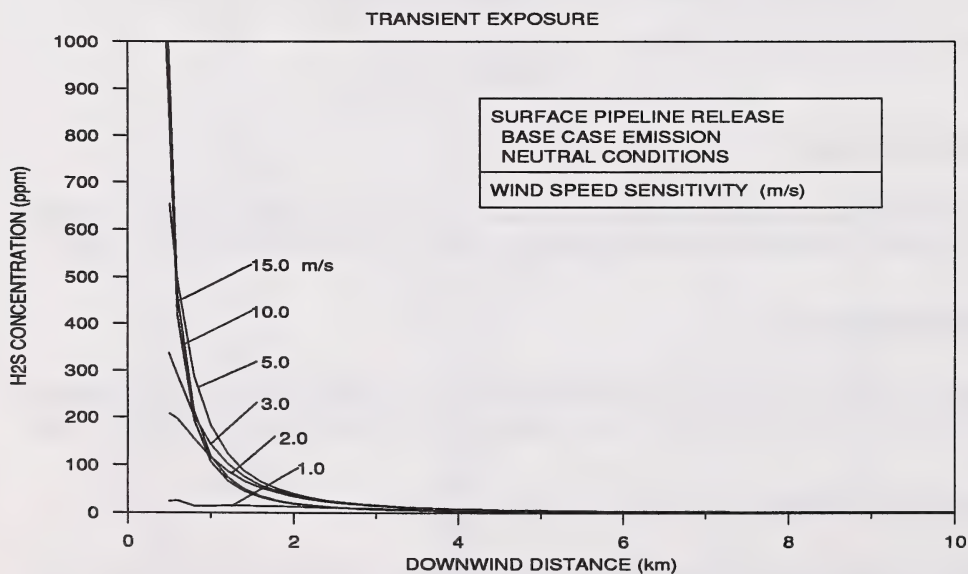


Figure 5.45

Predicted Peak H₂S Concentrations for Selected Wind Speeds (Neutral Conditions).

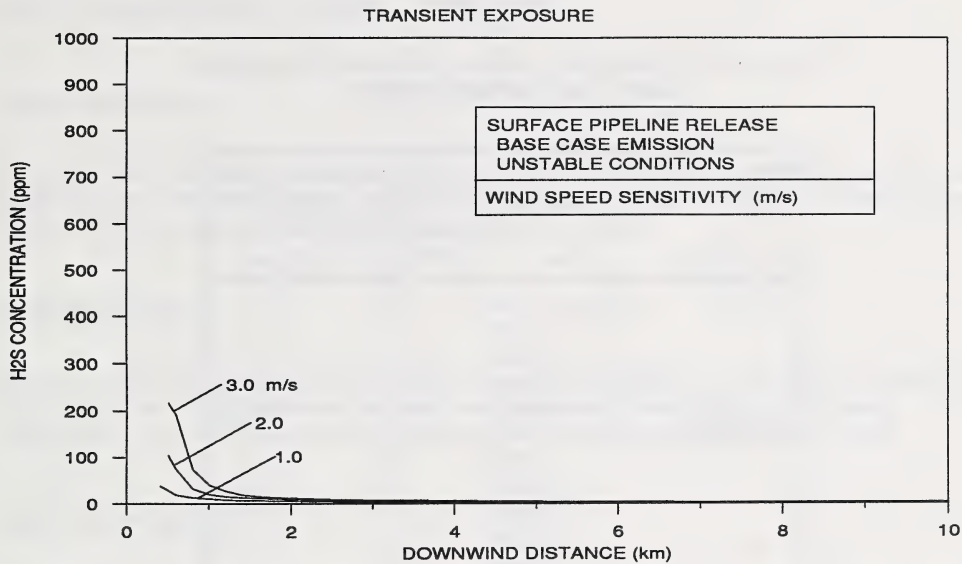


Figure 5.46

Predicted Peak H₂S Concentrations for Selected Wind Speeds (Unstable Conditions).

5.5.2 Hazard Zones

Distances to critical concentration values (potential hazard zones) are interpolated from the downwind distance concentration profiles. Table 5.30 summarizes the hazard zones associated with meteorology sensitivity runs.

The largest potential hazard zones are associated with:

- Low wind speeds for stable conditions
- Moderate wind speeds for neutral conditions
- Moderate wind speeds for unstable conditions

For large travel times, especially for the low wind speed stable conditions, the values must be used with caution.

Table 5.30

**Hazard Zone Sensitivity to Meteorological Parameters
(Base Case Pipeline Rupture).**

		Distance (km) to:	
Stability	Case	Transient H ₂ S	
		100 ppm	20 ppm
Stable	$U_{REF} = 1$ m/s	3.1	6.3
	2 m/s	2.5	6.3
	3 m/s	2.2	4.6
	5 m/s	1.4	2.7
Neutral	$U_{REF} = 1$ m/s	0.3	0.7
	2 m/s	1.1	2.6
	3 m/s	1.2	2.6
	5 m/s	1.3	2.7
	10 m/s	1.1	2.0
	15 m/s	1.0	1.9
Unstable	$U_{REF} = 1$ m/s	0.2	0.4
	2 m/s	0.5	1.0
	3 m/s	0.8	1.4

5.5.3 Probability of Lethality

Stable Conditions

The probability of lethality under the plume centreline versus downwind distance for stable conditions and four wind speeds is shown in Figure 5.47. From the graph it is evident that smaller wind speeds result in higher probabilities of lethality.

Neutral Conditions

Figure 5.48 shows the variation of the lethality curves with wind speed in neutral conditions. The maximum probabilities of lethality are associated with high wind speeds. The probabilities of lethality are strongly attenuated when compared to the stable cases.

Unstable Conditions

Figure 5.49 shows the lethality curves for three wind speeds in unstable conditions. Based on the relatively low predicted H₂S concentrations, the probability of lethality is estimated to be zero. Actually, the lethality decreases from 100% to 0% within several hundred metres of the well, but this resolution is not shown in the model output.

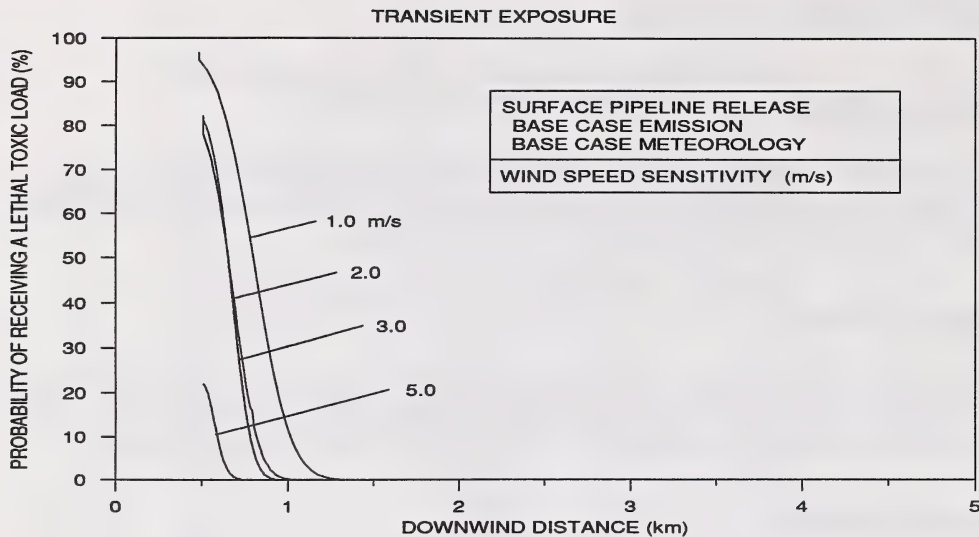


Figure 5.47

Predicted Lethality for Selected Wind Speeds (Stable Conditions).

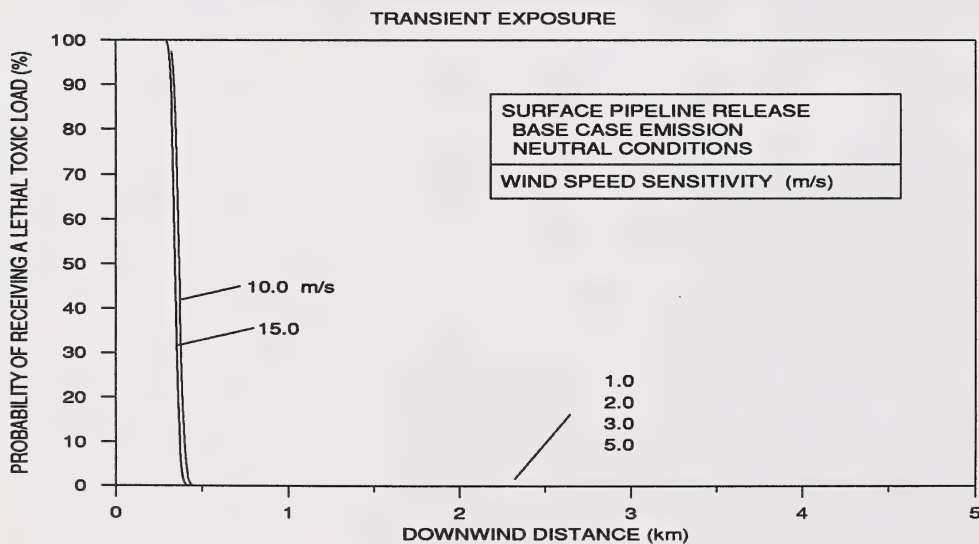


Figure 5.48

Predicted Lethality for Selected Wind Speeds (Neutral Conditions).

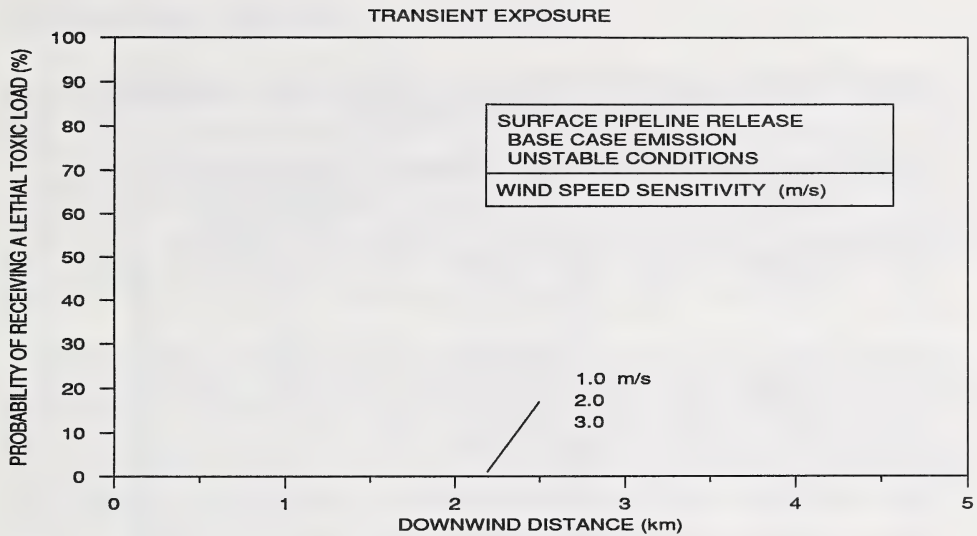


Figure 5.49

Predicted Lethality for Selected Wind Speeds (Unstable Conditions).

5.5.4 Potential Fatalities

Table 5.31 summarizes the potential number of fatalities associated with the various pipeline meteorology sensitivity runs. The largest potential number of fatalities for the horizontal base case release result from low wind speed stable conditions (2 potential fatalities) and high wind speed neutral conditions (1 potential fatality).

Table 5.31

**Potential Number of Fatalities Sensitivity to Meteorological Parameters
(Base Case Pipeline Rupture).**

Stability	Case	Potential Number of Fatalities
Stable	$U_{REF} = 1 \text{ m/s}$	2
	$U_{REF} = 2 \text{ m/s}$	1
	$U_{REF} = 3 \text{ m/s}$	1
	$U_{REF} = 5 \text{ m/s}$	0.1
Neutral	$U_{REF} = 1 \text{ m/s}$	0
	$U_{REF} = 2 \text{ m/s}$	0
	$U_{REF} = 3 \text{ m/s}$	0
	$U_{REF} = 5 \text{ m/s}$	0
	$U_{REF} = 10 \text{ m/s}$	1
	$U_{REF} = 15 \text{ m/s}$	1
Unstable	$U_{REF} = 1 \text{ m/s}$	0
	$U_{REF} = 2 \text{ m/s}$	0
	$U_{REF} = 3 \text{ m/s}$	0

5.6 Uncertainty Analysis

Air quality dispersion model calculations contain uncertainties which can be classified as those arising from reducible errors and those arising from inherent uncertainties (Fox, 1984). Reducible errors result from errors in source and meteorological input data and from limitations in the model physics. Inherent uncertainties result from the random nature of atmospheric turbulent motions that are responsible for the transport and diffusion processes. To provide a confidence level on the model predictions, it is desirable to quantify these uncertainties. In the absence of observations to allow direct uncertainty analysis, this quantification will be difficult to assess and will require subjective estimates.

Uncertainty analysis is relatively new and normally has not been included in dispersion modelling estimations. Regulatory agencies and decision makers usually assume that dispersion models provide a best estimate based on scientific principles and the addition of uncertainty analysis in the formal regulatory framework would be a difficult concept to incorporate. Most uncertainty analyses to date have been undertaken by modellers who wish to compare concentration observations to model predictions in order to evaluate the performance of their model.

5.6.1 Reducible Errors

Errors in the input source and meteorological data will propagate through the model and create an uncertainty in the model prediction. The limitations imposed by the model physics will also contribute to the uncertainty in the predicted value. An American Meteorological Society Workshop concluded that for modelling dispersion from tall stacks, the most potential for improvement in the predictions lies in the use of representative meteorological data and improved model physics (Fox, 1984).

For tall stacks, the source parameters are well defined since the stack is usually monitored on a routine basis. For an uncontrolled release, however, the definition of source parameters in advance of the event contains considerably more uncertainty. Basic errors are associated with the definition of the release rate, release geometry and gas composition. Often these parameters can be known with a better degree of confidence after the event. Even after the event, there may still be uncertainty in some of these parameters (e.g. Lodgpole flow rate, ERCB 1984).

Input errors related to meteorological data relate primarily to:

- The use of non-representative data for the area under study. This problem is magnified if the distance between the study area and the location of nearest meteorological station is large, if complex terrain is involved or if major differences in surface features in the area exist.
- The discretization of continuously varying meteorological parameters such as atmospheric stability (e.g. Pasquill Stability Classes A to F). This particular stability discretization is incorporated in various models (e.g. Alberta Environment, 1980; U.S. E.P.A. UNAMAP dispersion models).
- The errors in measuring, recording and archiving meteorological data.

Often meteorological models are used to compensate for the lack of meteorological data. For example, a power law wind profile model can be used to extrapolate a wind observation from one height to another.

A model, by definition, is a simplification of a real phenomenon and as a consequence, departures from the real world can be expected with any model. Some improvements in dispersion model physics that have been suggested to reduce these uncertainties are (Smith,1981; Fox,1984; Weil,1985):

- The incorporation of source dominated plume dilution near the release.
- The use of convective scaling to define turbulence in unstable boundary layers.
- The elimination of the "all-or-nothing" plume penetration model.
- The improvement of the Pasquill-Gifford plume dispersion coefficients by allowing stability to be continuous rather than discrete.
- The improvement of dispersion estimations under low wind speed conditions.
- The accounting for differences in the dispersion characteristics between surface and elevated releases.

The GASCON2 modelling system addresses the above concerns in an effort to reduce uncertainty in the model prediction. In particular, the model incorporates source modules which allow a wider variety of source conditions unique to well blowouts and pipeline ruptures than were previously available for models which were based on evaluating dispersion from stacks. Similarly, a meteorological preprocessor was designed to maximize the utility of available meteorological observations from standard AES stations. In addition, the dispersion model formulations used by GASCON2 attempt to incorporate our recent understanding on the physics of dispersion and all of the above mentioned improvements.

5.6.2 Inherent Uncertainties

Dispersion models are designed to predict a mean or ensemble-average value for a given set of atmospheric conditions. This given set of conditions is often defined by mean characteristics (e.g., mean wind speed, heat flux) which are known. Due to the random nature of atmospheric properties, however, the details of the atmospheric motion corresponding to this given set (as defined by mean values) are unknown. As a consequence, there will always be an uncertainty associated with a model prediction no matter how well the model mimics the behavior of the average physics of the atmosphere. This uncertainty is referred to as natural or inherent uncertainty (Fox, 1984).

Inherent uncertainties, to some extent, can also be related to the discretization process. The larger the size of the dispersion class, the larger the inherent uncertainty associated with model predictions for that class. This type of inherent uncertainty may be reduced by selecting smaller classes or a continuous distribution. In practise, decreasing the size of the class does not completely remove this type of contribution to the inherent uncertainty because observed data are usually grouped into discrete classes to facilitate data collection and evaluation.

Peak concentration estimates are required for flammability and toxicity estimates since the use of ensemble averages can be in error. These estimates require a probability function to be superimposed on the mean predicted value to account for the short time scale fluctuations.

5.6.3 Quantitative Estimation of Uncertainty

For elevated plume releases associated with unlimited mixing, the ground-level concentration below the plume centreline is estimated from:

$$\chi(x, 0, 0) = \frac{f\dot{m}_p}{\pi U_p \sigma_Y \sigma_Z} \exp\left[-\frac{(Z_p)^2}{2\sigma_Z^2}\right] \quad (5.1)$$

where $\chi(x, 0, 0)$ = concentration of a given plume component (H_2S or SO_2) at position $(x, 0, 0)$ (kg/m^3)

x = downwind distance from the rupture point (m)

f = fraction of the plume remaining below the mixed layer height

$\dot{m}_p$ = mass flow of the given plume component (H_2S or SO_2) in the release (kg/s)

U_p = wind speed at plume height (m/s)

σ_Y = standard deviation of the plume in the cross wind direction (m)

σ_Z = standard deviation of the plume in the vertical direction (m)

Z_p = height of the plume above ground level (m).

Standard error analysis statistics (e.g., Beers, 1962) can be used to show that the percent uncertainty in the predicted concentration, $\chi(x, 0, 0)$, can be estimated from:

$$\frac{\delta\chi}{\chi} = 100 \sqrt{\left(\frac{\delta\dot{m}_p}{\dot{m}_p}\right)^2 + \left(\frac{\delta U_p}{U_p}\right)^2 + \left(\frac{\delta\sigma_Y}{\sigma_Y}\right)^2 + \left[1 - \frac{Z_p^2}{\sigma_Z^2}\right]^2 \left(\frac{\delta\sigma_Z}{\sigma_Z}\right)^2 + \left[\frac{Z_p^2}{\sigma_Z^2}\right]^2 \left(\frac{\delta Z_p}{Z_p}\right)^2} \quad (5.2)$$

The above relationship evaluates random error and assumes that each parameter is independent and that the uncertainty in each parameter is normally distributed. Both $\dot{m}_p$ and U_p are independent of downwind distance whereas Z_p , σ_Y and σ_Z are dependent on downwind distance. In the above estimation of uncertainty, the fraction of the plume remaining in the mixing layer (f) was not assessed since it is clearly related to Z_p for unstable and neutral conditions, and is constant ($f = 1.0$) for stable conditions. Note that if the uncertainty in σ_Z is equal to the uncertainty in Z_p , Equation 5.2 is independent of the ratio Z_p/σ_Z .

To quantify the uncertainty associated with the GASCON2 model predictions, the following scenario was evaluated:

- Base case well blowout (Table 5.2).
- Base case gas composition (Table 5.5).
- Base case meteorology (Table 5.6).
- Relative uncertainties for the two cases given in Table 5.32.

Table 5.26 provides the relative uncertainty estimates for the two cases under consideration. Case 1 can be thought of as the case which has the smallest uncertainties associated with it. Case 2 represents a case with larger uncertainties. In both cases, the relative uncertainty for $\dot{m}_p$ was taken as 10%; it is recognized that the error in this value may be larger. The uncertainty values given in the table are subjective (arbitrary yet realistic) and are similar to those assumed by other investigators.

The predicted H_2S concentration values as a function of downwind distance are shown in Figure 5.28. The error band associated with each case indicates the relative uncertainty in the predicted values. The results can be summarized as follows:

- For Case 1, the uncertainty in the predicted H_2S concentrations are 38%. The corresponding uncertainty in the predicted distances to the 100 ppm and 20 ppm concentration values are 40% and 25%, respectively.
- For Case 2, the uncertainty in the predicted H_2S concentrations are 71%. The corresponding uncertainty in the predicted distances to the 100 ppm and 20 ppm concentration values are 75% and 80%, respectively.

As was previously mentioned, the Case 1 uncertainty values probably represent the best the model is able to predict with a given set of input parameters.

Table 5.32

**Relative Uncertainty Estimates (%) for Individual Parameters
(Irreducible and Inherent Uncertainty).**

Parameter	Case 1	Case 2
$\dot{m}_p$	10	10
U_p	10	15
σ_y	25	50
σ_z	25	50
Z_p	25	50
χ	38	71

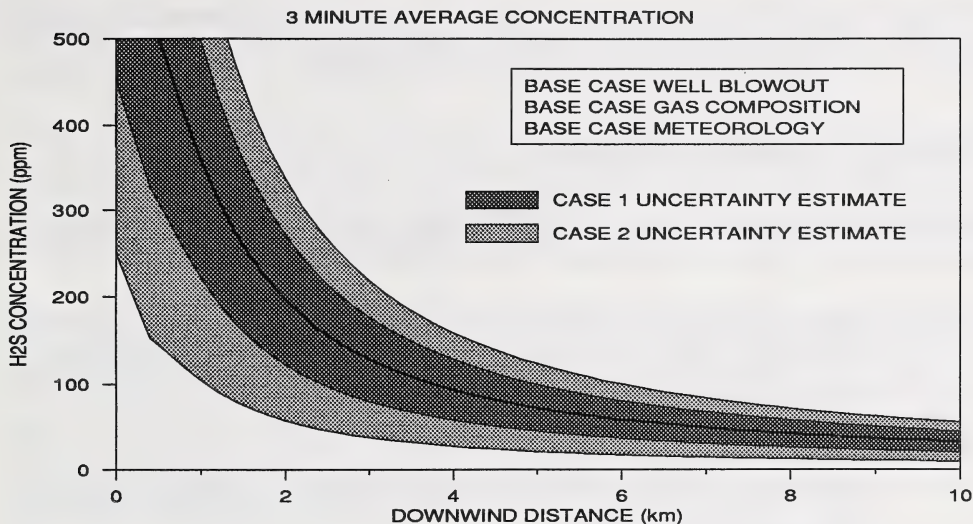


Figure 5.50

Estimated Uncertainty in the Prediction of H₂S Concentrations.

These estimated uncertainties are similar to those estimated by others for dispersion models. Specific examples from the literature include:

- A Monte Carlo simulation was undertaken to evaluate the uncertainty associated with Gaussian plume model predictions due to errors in the measurement of input parameters (Freeman *et al.* 1986). Their simulation indicated uncertainties of 30% for the ground-level concentration below the plume centreline for uncertainties of 20% in the following input parameters: Z_p , σ_y and σ_z .
- Smith (1981) provides rough estimates of the magnitude of uncertainties associated with Gaussian model predictions. These values range from 50% for a low level source to 200% for a tall stack.
- Pasquill and Smith (1983) fix a lower limit of 10% as attainable by the most ideal text book dispersion case. More realistic uncertainties are not expected "to be less than several tens of percent".
- Venketram (1979) estimated that inherent uncertainties can lead to uncertainties in the ensemble averaged value of up to 100% for dispersion estimates from tall stacks under unstable conditions.

At first glance, the magnitude of the uncertainties associated with dispersion model predictions may not be very comforting. It should be kept in mind, however, that concentration values in the atmosphere can vary by several orders of magnitude. It is anticipated that better decision making can arise from predictions that are within 50% than

can be developed in the absence of any data. The approach taken by the GASCON2 formulations attempts to maximize the utility of available data and our current understanding of the physics to minimize uncertainties in the model predictions.

5.7 Model Comparison Evaluation

The GASCON2 model formulations presented in Section 4 were compared to others which have been used in Alberta. In particular, the following modules were evaluated:

- *Transient Release Rate.* The double exponential blowdown model used was compared to a more rigorous non-isentropic non-ideal gas model to assess the capability of the former model to predict the high initial release rates (Section 5.7.1).
- *Plume Rise.* Predicted concentrations are sensitive to the height of the plume above the ground which is estimated from our understanding of plume rise processes (Section 5.7.2).
- *Plume Spread.* Predicted concentrations are also sensitive to the rate at which the plume spreads vertically and horizontally as it moves downwind (Section 5.7.3).
- *PLUMES2 Dispersion Model.* The Alberta Environment model PLUMES2 was used to calculate H₂S concentrations which result from a vertical steady-state well release. The results were compared to those predicted by GASCON2 (Section 5.7.4).
- *PUFF Dispersion Model.* The ERCB model was used to calculate H₂S concentrations which may result from a transient pipeline release. The results were compared to those predicted by GASCON2 (Section 5.7.5).

5.7.1 Transient Release Rate

The double-exponential pipeline blowdown model used by GASCON2 is described in Section 4.1.2. The Waterton pipeline rupture experiments conducted by APIGEC in 1978 showed excellent agreement between the double exponential and field data. However, for safety reasons, the Waterton studies were conducted using air rather than natural gas. Experience has shown that the one-dimensional, isentropic, compressible-flow, ideal-gas functions of classical thermodynamics work well for air. There was concern, however, whether this was true for sour gases containing H₂S and CO₂ which are noted for non-ideal phase behaviour. Pipeline releases are complex non-isentropic processes and it was thought presumptuous to assume that a simple model would be adequate to describe the blowdown.

A further study was conducted by Bishnoi (1986) to compare pipeline release rates for air (79% N₂ and 21% O₂) and for a sour gas (2.21% N₂, 10.52% CO₂, 31.80% H₂S, 54.66% CH₄ and 0.82% C₂H₆). The study used the Peng-Robinson equation of state (Peng and Robinson, 1976) to model the non-ideal gas behaviour and a mathematically rigorous method

(Picard, 1985) to solve the complex non-isentropic flow equations. The pipeline used for the comparison was 1250 m in length with an inside diameter of 154 mm. The initial gas conditions were 5500 kPa and 30°C.

The study showed that, unlike air, some condensation during the decompression occurred for the natural gas. The initial mass release for natural gas was slightly higher than for air. This seems intuitively correct due to the occurrence of condensation. The study further showed that non-ideal gas effects, although significant, would not preclude the use of ideal-gas functions from classical thermodynamics.

Figure 5.51 compares the estimated pipeline blowdown using non-ideal gas assumptions and rigorous mathematical modelling with that estimated using the double exponential model (ideal gas) employed by GASCON2. The same natural gas and pipeline parameters used in the Bishnoi study were used. The double-exponential model gives a somewhat higher release rate during the first 10 seconds following the rupture. It is during this period that the greatest departure from ideal gas behavior can be expected. Based on the comparison between the two models, it was judged acceptable to use the double-exponential model for dispersion modelling purposes.

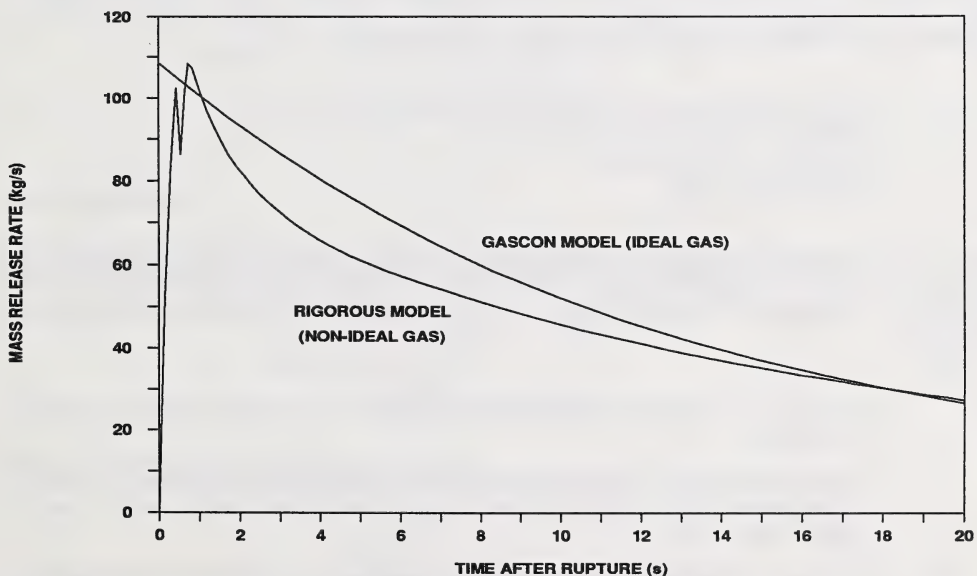


Figure 5.51

Comparison of Pipeline Rupture Mass Release Rates.

5.7.2 Plume Rise

The plume rise formulations used by Alberta Environment are based on the approach recommended by Briggs (1969). These formulations, in many cases, are different than the Briggs approach employed by GASCON2 as plume rise termination criteria. Tables 5.33 and 5.34 summarize the plume rise approach adopted by Alberta Environment (referred to as the Briggs 1969 approach) for buoyant (Δh_B) and momentum jet (Δh_M) plumes, respectively. The final rise is given as the larger of Δh_B and Δh_M .

The following assumptions were made for the comparison between the model plume rise predictions and those predicted through the use of the Briggs 1969 approach:

- Vertical jet ($\lambda = 90^\circ$)
- Steady state flow rate ($260 \cdot 10^3 \text{ m}^3/\text{d}$)
- Release diameter (62.0 mm)
- Gas temperature (40.0°C)
- Base Case gas properties (Section 5.1.3)
- Ambient temperature (0°C)
- Surface roughness (0.10 m).

The Briggs 1969 approach requires exit velocities and gas density in order to evaluate plume rise. For the purposes of comparison, the GASCON2 predicted values at the "q" plane (Figure 4.2) were used as input to the Briggs 1969 approach:

- Exit velocity of gas (341.6 m/s) (sonic assumption)
- Effective release diameter (110 mm)
- Gas density (0.997 kg/m^3)
- Stack height (1 m).

Figure 5.52 compares the predicted final plume rises using the GASCON2 formulations with those using the Briggs 1969 approach for unignited releases under unstable and neutral atmospheric conditions. From the figure and the associated computer print out it can be observed:

- The Briggs' 1969 approach does not differentiate between neutral and unstable conditions.
- The predicted plume rise values using the two approaches are similar for neutral atmospheres with GASCON2 predicting lower plume rise for wind speeds greater than 2 m/s.
- For neutral conditions, the plume height predicted by GASCON2 is limited by the plume penetration criteria for a wind speed of 1 m/s; for higher wind speeds, the plume height is limited by the Briggs' criteria.
- The values predicted by GASCON2 for unstable conditions are less than the Briggs 1969 values for wind speeds less than 3 m/s and more than the Briggs 1969 values for wind speeds greater than 3 m/s.
- For unstable conditions, the plume height predicted by GASCON2 is a very weak function of the mixing height Z_i specified by the user. More importantly, plume rise cannot exceed Z_i .

Table 5.33

Briggs 1969 Method for Estimating Buoyant Plume Rise.

Unstable and Neutral Conditions

Following the Briggs 1969 approach, the final plume rise is given by:

$$\Delta h_B = \frac{1.6 F_B^{1/3} x_F^{2/3}}{U_{ST}} \quad (5.3)$$

where: F_B = buoyancy flux as defined in Table 4.4 (m^4/s^3)
 U_{ST} = wind speed at stack height (m/s) = U_{REF}

For ignited conditions, F_B is given by $F_B = 0.75(0.000037)Q_H$ where Q_H = heat released by the combustion of gases (calories/s). The 0.75 factor allows for a 25% radiation loss.

The plume is assumed to level off at a distance x_F given by:

$$\begin{aligned} x_F &= 49 F_B^{5/8} & \text{for } F_B &\leq 55 \text{ m}^4/\text{s}^3 \\ x_F &= 119 F_B^{2/5} & \text{for } F_B &> 55 \text{ m}^4/\text{s}^3 \end{aligned} \quad (5.4)$$

Stable Conditions

For a stable atmosphere, the plume is predicted to level off at a height of:

$$\Delta h_B = 2.6 \left(\frac{F_B}{U_{ST} S} \right)^{1/3} \quad (5.5)$$

where S is the stability parameter defined by:

$$S = \frac{g}{T_A} \frac{\partial \theta}{\partial Z} \quad (5.6)$$

where: g = acceleration of gravity (9.81 m/s^2)
 T_A = ambient air temperature (K)
 $\partial \theta / \partial Z$ = vertical potential temperature gradient (K/m)
 $= 0.04 \text{ (K/m)}$

Table 5.34

Briggs 1969 Method for Estimating Momentum Jet Plume Rise.

Unstable and Neutral Conditions

The final rise is given by:

$$\Delta h_M = 6 \frac{V_{ST}}{U_{ST}} r_{ST} \quad (5.7)$$

where:

V_{ST} = exit speed of the effluent (m/s)

r_{ST} = radius of the stack (m)

U_{ST} = wind speed at stack height (m/s) = U_{REF}

Stable Conditions

The final rise is given by:

$$\Delta h_M = 1.5 \left(\frac{F_M}{U_{ST}} \right)^{1/3} S^{-1/6} \quad (5.8)$$

where:

F_M = momentum flux defined in Table 4.4 (with $\lambda = 90^\circ$)

S = the stability parameter defined by Equation 5.6.

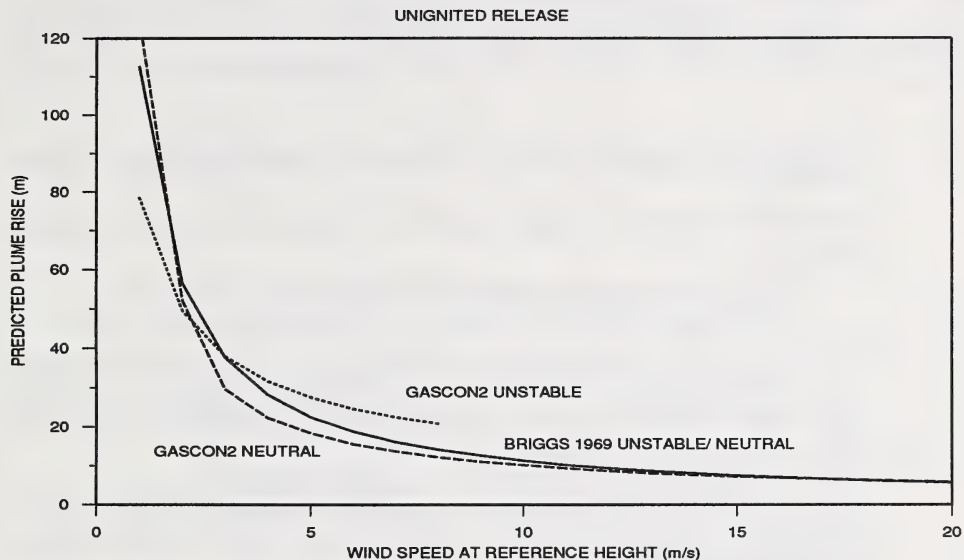


Figure 5.52

**Comparison of GASCON2 and Briggs 1969 Final Plume Rise
for Neutral and Unstable Conditions
(Unignited Release).**

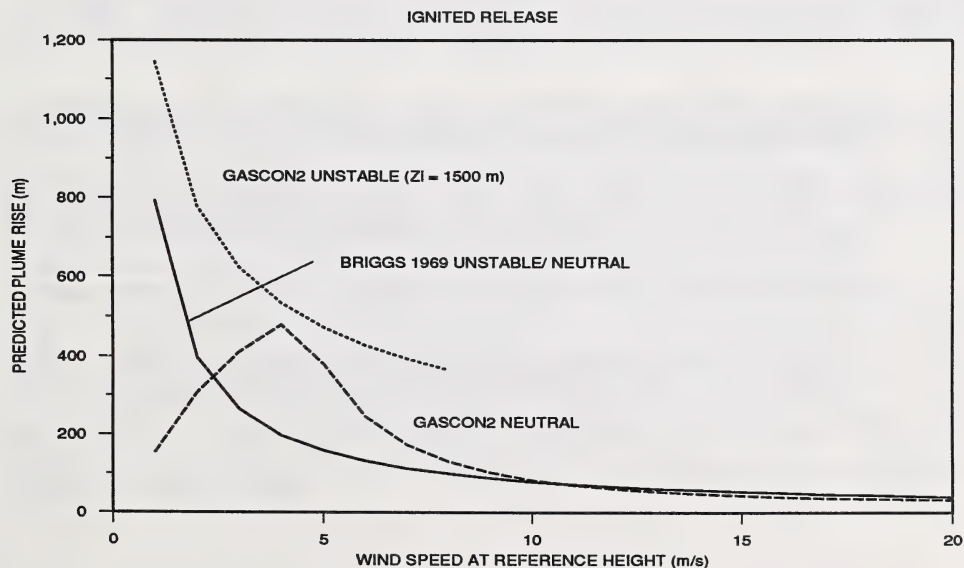


Figure 5.53

**Comparison of GASCON2 and Briggs 1969 Final Plume Rise
for Neutral and Unstable Conditions
(Ignited Release).**

Figure 5.53 compares the predicted final plume rises using the GASCON2 formulations with those using the Briggs 1969 approach for ignited releases under unstable and neutral atmospheric conditions. From the figure and the associated computer print out it can be noted that:

- The Briggs 1969 approach does not differentiate between neutral and unstable conditions.
- For neutral conditions, the plume height predicted by the GASCON2 model is limited by:
 - the plume penetration criteria for wind speeds of 1 to 4 m/s
 - the Briggs' plume rise criteria for wind speeds greater than 5 m/s.

The combination of the above plume rise levelling off criteria results in a plume rise - wind speed profile that differs from the Briggs 1969 approach. For wind speeds greater than 10 m/s, the two approaches are in agreement with each other.

- The values predicted by GASCON2 for unstable conditions assume a mixing height value (Z_i) of 1500 m. For this unstable case, the transition from unstable to neutral atmospheres takes place at a wind speed of 8 m/s. Predicted plume rise cannot exceed Z_i .
- For unstable cases with a mixing height of 100 m, the predicted GASCON2 plume heights are forced to 100 m by the plume penetration criteria. For this unstable case, the transition from unstable to neutral atmospheres takes place at a wind speed of 3.2 m/s.

Figure 5.54 compares the predicted final plume rises using the GASCON2 formulations with those using the Briggs 1969 approach for stable atmospheric conditions. From the figure and the associated computer print out it can be noted that:

- For the unignited and ignited releases, the values predicted by the GASCON2 model and the Briggs 1969 show a similar trend.
- The predicted final plume rise for the unignited releases are dominated by vertical momentum whereas the ignited releases are dominated by buoyancy. The predicted momentum dominated plume rises for the example shown in the figures are generally much less than those which are dominated by buoyancy.
- GASCON2 predicted plume rises are higher due to the calculation of the buoyancy flux at the "S" or "C" plane where air has been entrained.

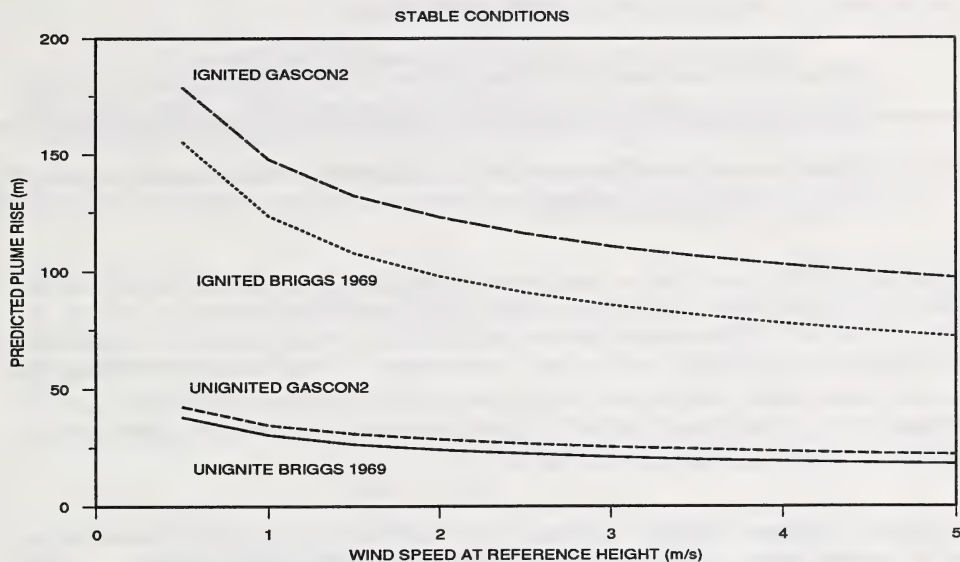


Figure 5.54

Comparison of GASCON2 and Briggs 1969 Final Plume Rise for Stable Conditions (Unignited and Ignited Releases).

5.7.3 Plume Spread

Plume spread values (σ_y and σ_z) determine the rate of dilution as the plume moves downwind. The plume spread formulations used have been documented in Sections 4.5.4 and 4.5.5 of this report. The selected formulations allow for the prediction of a continuous range of σ_y and σ_z values for any given set of atmospheric conditions (PBL parameters). The GASCON2 formulations differentiate between surface and elevated plumes.

The GASCON2 σ_y and σ_z formulations differ from those used by Alberta Environment (1980). Alberta Environment estimates σ_y and σ_z values for six discrete Pasquill dispersion classes ranging from extremely unstable (A) through neutral (D) to moderately stable (F). This method (as given in Table 5.35) is based on formulations given by Smith (Pasquill, 1983) for σ_z and a power law fit to the Pasquill-Gifford values (Turner, 1970) for σ_y . The associated plume spreads are referred to as the Pasquill-Smith plume spreads. The plume spread values are a function of Pasquill stability class, downwind distance, surface roughness and (for σ_y) averaging period.

For the purposes of comparison, the following were assumed:

- Horizontal spreads were normalized to three minute averaging periods through the use of the power law relationship (Equation 4.134). The GASCON2 horizontal plume spread values correspond to a 30 minute averaging period.
- Virtual point source effects were not included to remove the source dependency.
- A surface roughness of 0.10 m.

Since the GASCON2 model does not use discrete dispersion classes like the Pasquill-Smith approach, the plume spread values, where applicable, are given as a range of values. In addition, GASCON2 differentiates between surface and elevated releases for horizontal plume spreads under unstable and neutral atmospheres. Under stable conditions, the horizontal plume spreads are the same but depend on the elevation of the plume (Z_p or $\bar{Z}$) with respect to the mixing layer height Z_i . For surface releases, the vertical plume spreads presented are $\bar{Z}$, the mean height of the plume.

For unstable conditions (Figures 5.55 and 5.56), GASCON2 generally estimates larger values of vertical plume spread and smaller values of horizontal plume spread. Lower plume spreads are associated with higher wind speeds, thus a range is presented (1 to 3 m/s). The horizontal spread associated with surface releases is less than that for elevated releases.

For neutral conditions (Figures 5.57 and 5.58), GASCON2 estimates similar values of vertical plume spread and smaller values of horizontal plume spread. The plume spreads are independent of the wind speed. The horizontal spread associated with surface releases is larger than that for elevated releases at distances of less than 500 m. For similar conditions, the use of the GASCON2 plume spreads values are expected to produce ambient concentrations larger than those associated with the use of the Pasquill-Smith plume spread values.

For stable conditions (Figures 5.59 and 5.60), GASCON2 estimates similar values of vertical and horizontal plume spreads. Plume spreads depend on the elevation of the plume with respect to the mixing height Z_i . Lower plume spreads are associated with higher elevations. The plume spreads also decrease to a minimum value with windspeed. For example, the plume spreads at 3 m/s are essentially the same as for 1 m/s. The range shown corresponds to 1 to 5 m/s and plume elevations from ground level to Z_i .

Table 5.35

Pasquill-Smith Method for Estimating Plume Spreads.

Following the Pasquill-Smith Method for Estimating Plume Spreads. Pasquill-Smith formulations, the vertical spread for a plume in a boundary layer of known stability is:

$$\sigma_Z = \sigma_{ZREF} \left(\frac{x}{x_{REF}} \right)^{P_Z} \quad (5.10)$$

and the cross wind spread is:

$$\sigma_Y = \sigma_{YREF} \left(\frac{x}{x_{REF}} \right)^{P_Y} \left(\frac{t_{AVG}}{180} \right)^{0.2} \quad (5.11)$$

where

x_{REF} = reference distance = 1000 m

x = downwind distance (m)

t_{AVG} = averaging period (s)

P_Z, P_Y = powers which depend on boundary layer stability and roughness length

$\sigma_{ZREF}, \sigma_{YREF}$ = reference plume spreads which depend on boundary layer stability and roughness length (m)

For a surface roughness (Z_0) of 0.1 m, the values for σ_{ZREF} , P_Z , σ_{YREF} and P_Y are as given below:

Stability Class	σ_{ZREF} (m)	P_Z	σ_{YREF} (m)	P_Y
A	140	0.90	210	0.88
B	80	0.85	160	0.88
C	56	0.80	100	0.88
D	38	0.76	68	0.88
E	23	0.73	50	0.88
F	12	0.67	34	0.88

The vertical plume spread is considered independent of averaging time. The horizontal plume spread, however, is considered valid for a three-minute averaging time.

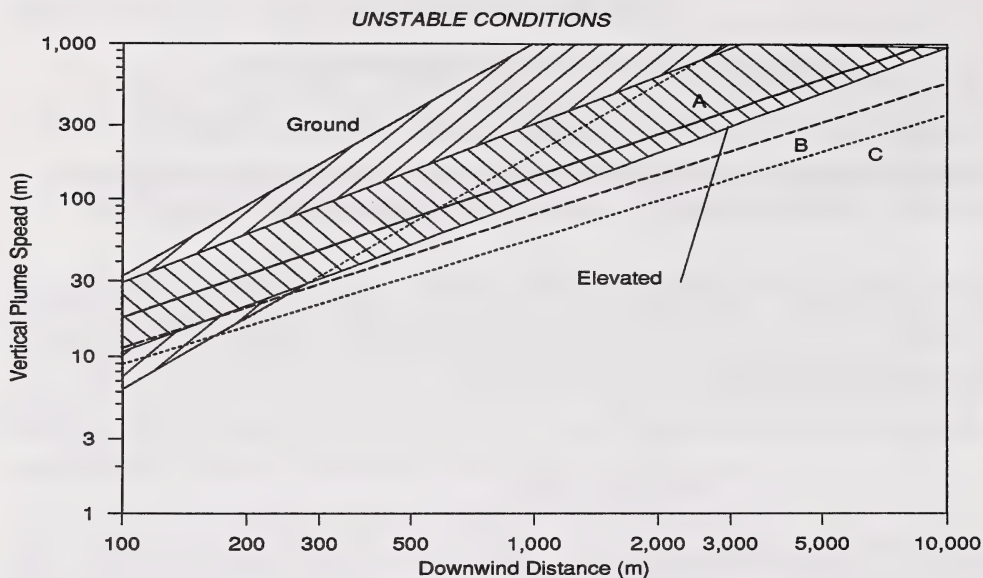


Figure 5.55

**Comparison of GASCON2 and Pasquill-Smith Vertical Plume Spread
for Unstable Conditions.**

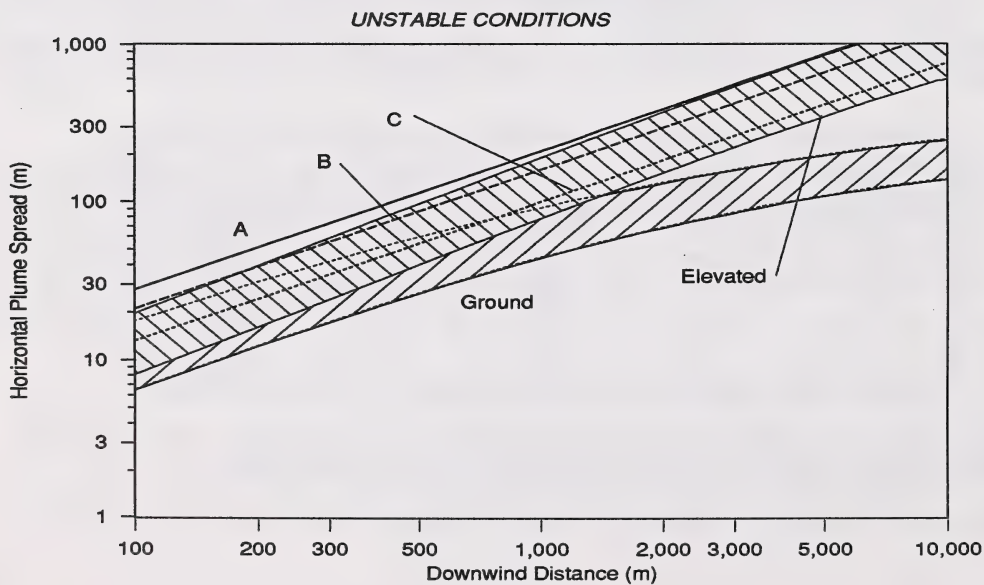


Figure 5.56

**Comparison of GASCON2 and Pasquill-Smith Horizontal Plume Spread
for Unstable Conditions.**

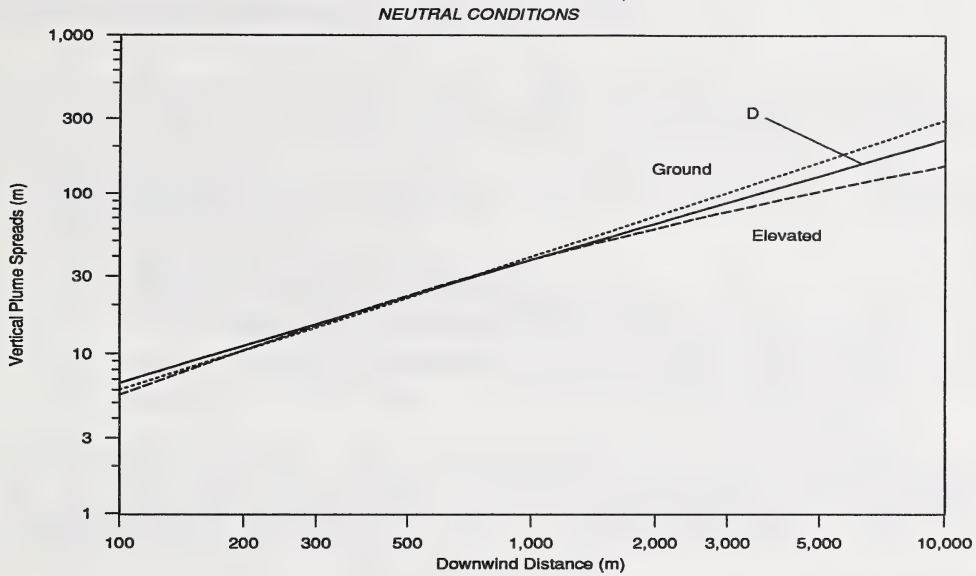


Figure 5.57

**Comparison of GASCON2 and Pasquill-Smith Vertical Plume Spread
for Neutral Conditions.**

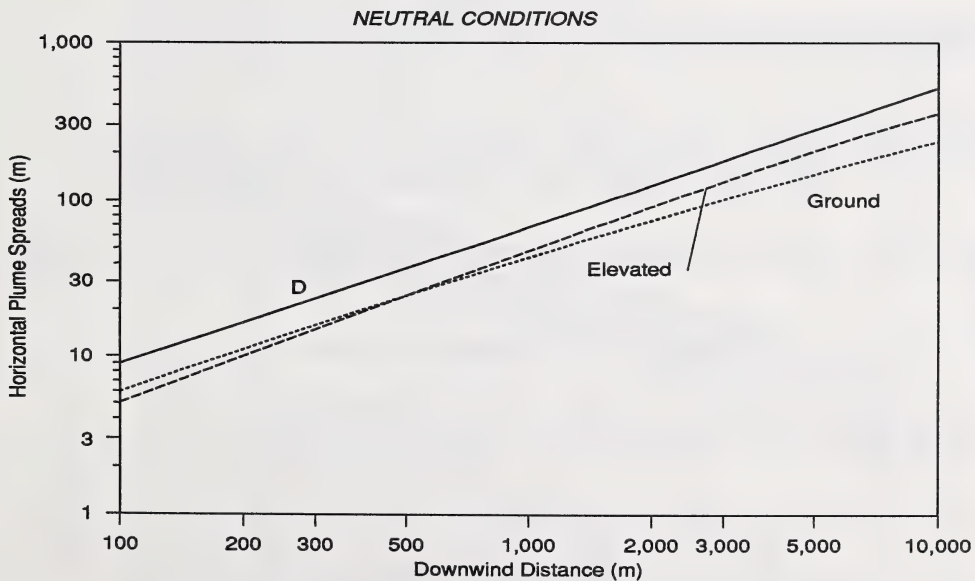
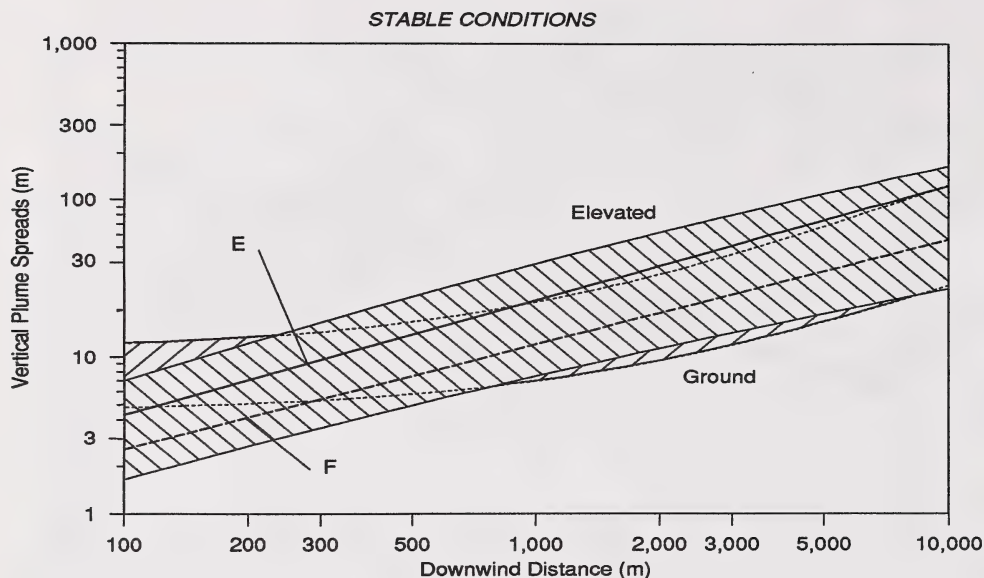
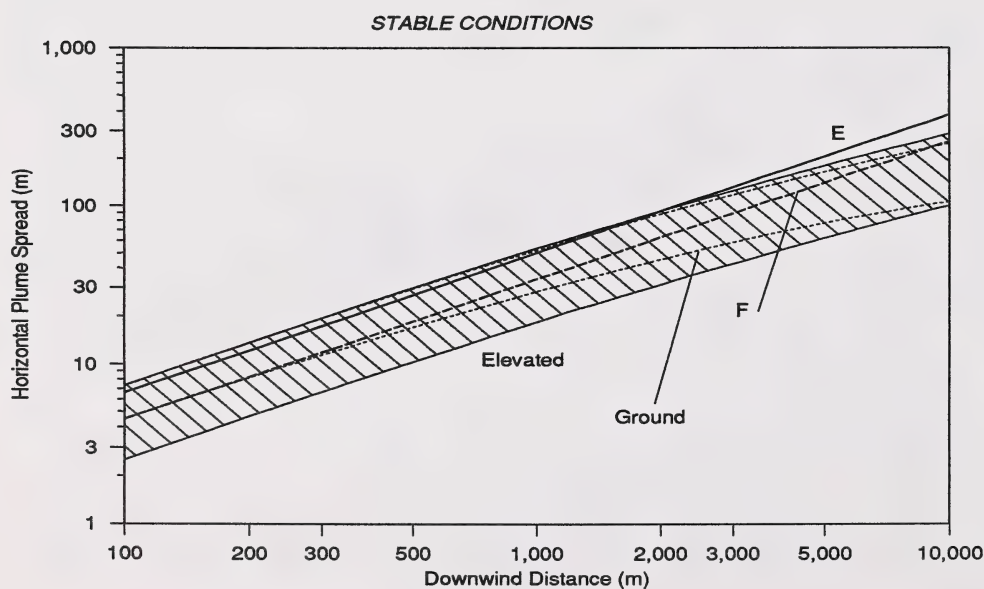


Figure 5.58

**Comparison of GASCON2 and Pasquill-Smith Horizontal Plume Spread
for Neutral Conditions.**



**Comparison of GASCON2 and Pasquill-Smith Vertical Plume Spread
for Stable Conditions.**



**Comparison of GASCON2 and Pasquill-Smith Horizontal Plume Spread
for Stable Conditions.**

5.7.4 PLUMES2 Dispersion Model

The Alberta Environment dispersion model PLUMES2 is a generalized flat terrain Gaussian plume model which uses the Briggs 1969 plume rise relationships (Tables 5.33 and 5.34) and the Pasquill-Smith plume spread values (Table 5.35) (Alberta Environment, 1988).

For the purposes of comparison, the following scenario was evaluated using the PLUMES2 and GASCON2 models:

- Unignited and ignited well blowout.
- Modified base case well blowout as given in Section 5.7.2 (vertical jet).
- A modified base case meteorology as given in Table 5.6 (wind speed values of 2 m/s and 3 m/s were used).

The above modifications were made since the Briggs 1969 plume rise formulations are only applicable to vertical releases (Section 5.7.2) and the Pasquill stability class is not defined for stable conditions when the wind speed is less than 2 m/s. Stability class F was used for the PLUMES2 model predictions.

Figure 5.61 compares the predicted H₂S concentrations from the two models. The figure indicates the following:

- For a 2 and 3 m/s wind speeds, the peak concentrations predicted by GASCON2 are about double that predicted by PLUMES2.
- The GASCON2 model predicts a potential hazard zone (defined by the 20 ppm concentration) which is about double that predicted by PLUMES2 for 2 m/s winds.
- For stable conditions and the unignited release scenario considered, it appears that GASCON2 is more conservative than PLUMES2. That is, GASCON2 predicts higher concentrations and larger potential hazard zones.

Figures 5.62 compares the predicted SO₂ concentrations from the two models. The figure indicates the following:

- The PLUMES2 model predicts the same SO₂ concentrations for the 2 and 3 m/s wind speeds.
- GASCON2 predicts a much lower SO₂ concentration with 2 m/s wind speeds than with 3 m/s wind speeds due to a higher plume rise and lower plume spreads associated with the 2 m/s winds.
- For a 2 m/s wind speed, PLUMES2 predicts higher concentrations than GASCON2.
- For a 3 m/s wind speed, GASCON2 predicts higher concentrations than PLUMES2 for distances beyond 5 km.

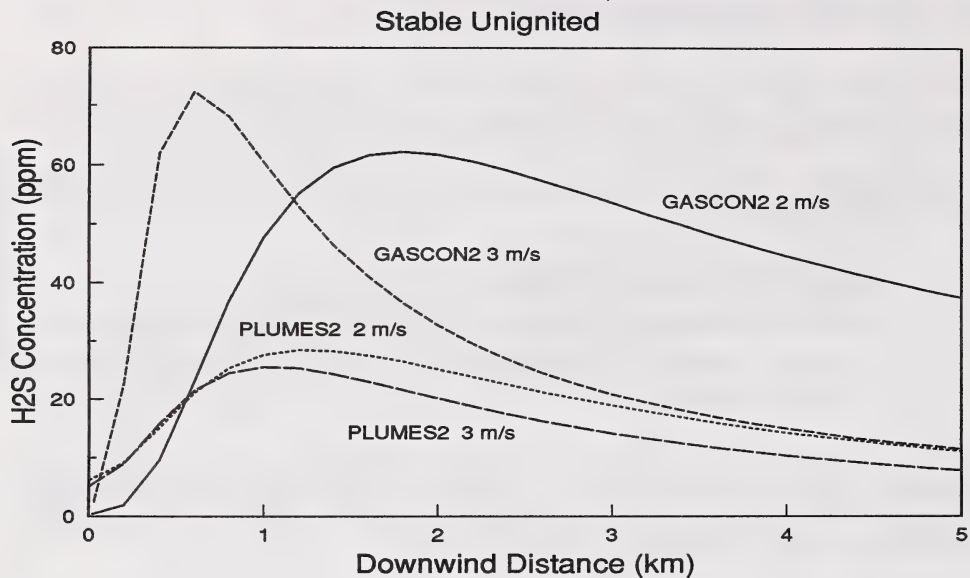


Figure 5.61

Comparison of Predicted GASCON2 and PLUMES2 H₂S Concentrations.

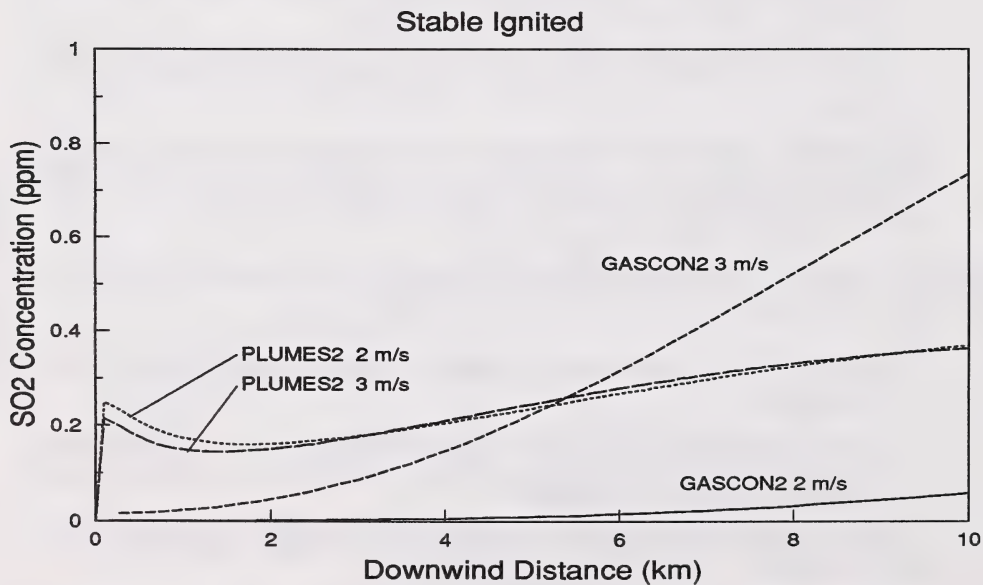


Figure 5.62

Comparison of Predicted GASCON2 and PLUMES2 SO₂ Concentrations.

5.7.5 PUFF Dispersion Model

The ERCB PUFF model was developed to estimate ground-level H_2S concentrations from transient pipeline releases (ERCB, 1979). The model assumes that the pipeline gas is released as a series of discrete puffs, each with a mass δm released over a period δt . Each puff is allowed to spread in three dimensions as it is carried downwind. The resulting ground-level concentrations are estimated from the numerical superposition of all the puffs. This model, which is often called an integrated puff model (e.g. Peterson *et al.* 1984), incorporates the following assumptions:

- The puffs have a Gaussian distribution in three dimensions (σ_x , σ_y and σ_z).
- The along-wind spread (σ_x) equals the lateral spread (σ_y).
- The Pasquill-Smith plume spreads are used to estimate the vertical (σ_z) and lateral (σ_y) puff spreads.
- Lateral plume spreads are estimated using the three minute average σ_y values.
- A power law vertical wind speed profile is incorporated in the model.

Since the ERCB PUFF model does not estimate release rates or plume heights, the time profiles of these values are required as input parameters. For the comparison evaluation, these time profiles were obtained from the GASCON2 model output. Similarly, the power law wind profile exponent was also taken from the GASCON2 output. The PUFF model has the option of incorporating an initial dilution factor. For this evaluation, no initial dilution was assumed.

For the purposes of comparison, the following scenario was evaluated using the PUFF and GASCON2 models:

- Unignited pipeline rupture.
- Base case pipeline rupture as given in Table 5.4.
- Base case gas composition as given in Table 5.5.
- A modified base case meteorology as given in Table 5.6 (the wind speed was increased from 1 to 2 m/s).

The above modification was made since the Pasquill stability class is not defined for stable conditions when the wind speed is less than 2 m/s.

Figure 5.63 compares the predicted H_2S concentrations from the two models. The figure indicates the following:

- The downwind concentration profiles are similar for both models.
- The downwind distances from the pipeline rupture to the exposure zone (defined by the 100 ppm concentration) are similar for both models.
- The main differences occur between the predictions by the two models near the pipeline rupture point.

- The initial investigations presented here indicate that the predictions by GASCON2 and PUFF are similar. This is not that surprising since the GASCON2 release rate and plume height profiles were used as input into the PUFF model, with only the plume spreads differing.

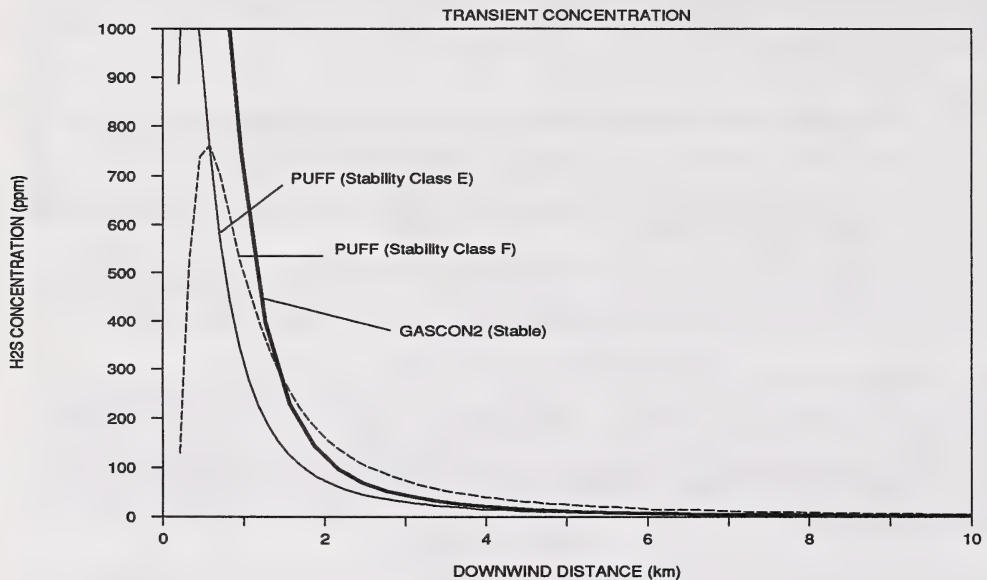


Figure 5.63

Comparison of Predicted GASCON2 and PUFF H₂S Peak Concentrations.

5.8 Comparison With Observations

Data on downwind H₂S and SO₂ concentrations from natural gas pipeline bursts are unavailable. Some observations, however, are available from three well-known well blowouts in Alberta (Lodgepole, Claresholm and Rainbow Lake). This section presents a brief description of each blowout, the available data and the comparison with GASCON2 predictions.

Due to the severe limitations of the data associated with each blowout, this comparison exercise should **not** be viewed as a model verification or validation exercise. The air quality data associated with each blowout were collected with public safety interests in mind and not for model verification or validation purposes. As a consequence, most of the observations are poorly documented with respect to magnitude, location and averaging time. In addition, no effort was made to collect concurrent meteorological observations which are essential input parameters for any plume dispersion model. The exercise here should only be viewed with providing a preliminary indication of the model performance.

The model concentration data which were used in this comparison were selected to meet the following general criteria:

- The location of the monitor during the concentration observation had to be clearly documented. This criterion refers specifically to mobile monitors.
- Only concentration observations within 25 km of the well blowout were considered. This criterion recognizes the distance limitation of dispersion models.
- Only significant concentration observations were considered. The selection of the level of significance was subjective and varied for each well blowout considered. The selection of significant events will bias the observation data set to large concentration values.
- Only concentration observations which could be related to a clearly documented averaging period were selected.

The above criteria were selected in an effort to produce a reasonably large data set. The scope of this study precluded a rigorous comparison of model predictions with all observations. The adoption of the above selection criteria produced 50 concentration observations (43 H₂S values and 7 SO₂ values) for the comparison. Most of the observations were associated with the Lodgepole well blowout (45 values).

5.8.1 Lodgepole Well Blowout

The Amoco-Dome Brazeau River well is located about 20 km west of Lodgepole amid rolling forested terrain. The blowout occurred when reservoir fluids unexpectedly entered the well bore during the drilling of the well.

The uncontrolled release began at 14:30 on October 17, 1982 and was not brought under control until 15:53 on December 23, 1982. During this period there were four distinct emission regimes:

- 14:30 October 17 to 14:15 November 1
Sour gas was escaping from a drill pipe which protruded 0.3 m above the rotary table on the drill rig. During this period a portion of the escaping gas was deflected by the overhead drill rig structure. The escaping gas was unignited.
- 14:15 November 1 to 10:50 November 14
Some gas was accidentally ignited; the drill rig was destroyed; all debris was removed; and finally the flame was extinguished. Gas was vented to the atmosphere through the intermediate casing.
- 10:50 November 14 to 13:25 November 25
Unignited sour gas was escaping from the intermediate casing at essentially ground level. A vertical plume with no deflection resulted. Gas was vented to the atmosphere through the intermediate casing.
- 13:25 November 25 to 15:53 December 23
The sour gas was accidentally ignited again and remained ignited until the well was brought under control. Gas was vented to the atmosphere through the intermediate casing.

Estimated well blowout parameters are summarized in Table 5.36. The two flow rates in the table refer to the maximum flow rates which were possible through the drill tube and the intermediate casing.

Seven stationary and five mobile units collected various combinations of H_2S , SO_2 and wind data within a 50 km radius of the Lodgepole well. Further monitoring observations were rejected due to ambiguous reporting and limited analyzer ranges. Air quality data used for the model comparison were obtained from the Lodgepole and Cynthia stationary units and from the Alberta Environment mobile unit.

Table 5.37 summarizes the maximum observed H_2S and SO_2 concentrations from the mobile units. These maximum values represent the maximum concentration associated with a monitoring event defined as a series of values over limited time duration where the mobile monitor was in the same or similar location. The selection of each monitoring event was subjective and dependent on the monitoring unit. For the stationary units, the values shown in the table represent one-hour averaging periods. For the mobile unit, the reported peak concentrations are assumed to be representative of fifteen second averaging periods. These observed values presented in the table have all been normalized to an averaging period of three minutes through the use of a power law relationship.

Petro-Canada Resources maintained and operated a meteorological monitoring site 12 km west-southwest of the well site during the blowout. Wind data are available from a 20 m tower which was located within a clearing (approximate diameter 300 m) (Morrow and Murray, 1983). The wind ($Z_{REF} = 20$ m) and temperature data given in Table 5.31 represent hourly average values observed at the station. Cloud and snow cover data were obtained from AES hourly data records for Edson. The table also provides the meteorological preprocessor predictions for surface heat flux (H_o), stability and mixing height (Z_i). The surface roughness length used was estimated from the nature of the terrain surrounding the blowout site: for Lodgepole (rolling forested terrain) Z_o was assumed to be 1.0 m.

5.8.2 Claresholm Well Blowout

The Consolidated Pipeline Ltd. and Drummond et al. Claresholm well is located about 13 km east of the town of Claresholm amid flat tree-less terrain. During an attempt to remove a hydrate plug, the well head failed due to a complete break below the master valve.

The uncontrolled release of gas began at 18:45 on September 24, 1984 and ended at 11:45 on September 28, 1984. Prior to the removal of the well head assembly at 15:00 on September 25, 1984, the vertical rise of the escaping gases was partially obstructed. The estimated plume rise prior to well head removal was 10 m (based on candid photographs). After the well head was removed, a well-defined vertical jet resulted (typical plume rise estimate of 25 m as observed from candid photographs). During the entire period the well remained unignited. Well blowout parameters are summarized in Table 5.36.

Table 5.36
Source Parameters for Selected Well Blowouts.

Parameter	Lodgepole	Claresholm	Rainbow Lake
Location			
Legal	13-12-48-12W5M	6-30-12-25W4M	7-34-107-10W6M
Latitude (°N)	53.16	50.04	85.33
Longitude (°W)	115.66	113.40	119.45
Elevation (m)	945	985	460
Flow Rate			
Total (10 ³ m ³ /d)	2830	226	204
Total (kg/s)	36.1 (4250)*	2.42	2.42
Gas Properties			
Molecular Weight (kg/kmole)	26.2	21.9	24.3
Specific Heat Capacity (J/(kg K))	1662	1768	1641
Heat of Combustion (MJ/m ³)	38.1	33.2	33.5
H ₂ S content (mole %)	25.0	1.0	23.1
C ₁ content (mole %)	56.0	77.6	60.2
Release Conditions			
Height (m)	7.0 (1.0)*	1.0	4.0
Diameter (mm)	97.2 (216.8)*	62.0	62.0
Temperature (°C)	60.0	27.0	40.0

* From 14:10 Nov 1 1982 to 15:53 Dec 23 1982.

Table 5.37

Observed H₂S and SO₂ Concentrations and Associated Meteorological Parameters for the Selected Well Blowouts.

No.	DATE	TIME	CLOUD COVER	SNOW COVER	U_{REF}	T_A	H_o	Z_i	MONITOR		OBSERVED		PREDICTED	
			(%)		(m/s)	(°C)	(W/m ²)	(m)	TYPE	DIST	H ₂ S	SO ₂	H ₂ S	SO ₂
										(km)	(ppm)	(ppm)	(ppm)	(ppm)
1	OCT 18 82	9:40	10	Yes	1.4	-8	-25	S	69	M	21	7.3	67.5	
2	OCT 20 82	10:00	60	Yes	1.7	-9	-13	S	78	L	21	2.2	27.7	
3	OCT 20 82	24:00	0	Yes	2.5	-3	-27	S	97	L	21	3.1	13.7	
4	OCT 21 82	10:00	20	Yes	0.8	-7	-22	S	49	L	21	2.7	33.3	
5	OCT 26 82	22:00	50	No	1.9	6	-15	S	83	L	21	3.6	23.6	
6	OCT 27 82	2:22	10	No	3.3	-1	-25	S	199	M	21	6.1	7.9	
7	OCT 27 82	6:00	20	No	2.8	0	-22	S	104	C	22	3.0	10.7	
8	OCT 29 82	12:00	30	No	1.7	-1	68	U	85	C	22	4.3	4.6	
9	OCT 29 82	20:00	20	No	1.9	-2	-22	S	83	M	21	8.5	41.9	
10	OCT 29 82	22:15	0	No	2.5	-3	-27	S	97	M	18	9.1	28.5	
11	OCT 30 82	20:35	10	No	2.2	-3	-25	S	90	M	21	7.3	31.6	
12	OCT 31 82	4:00	50	No	2.5	-3	-15	S	97	C	22	1.2	13.1	
13	OCT 31 82	23:55	90	No	3.1	2	-5	N	711	M	21	8.5	4.3	
14	OCT 31 82	24:00	90	No	3.1	2	-5	N	711	L	21	1.4	2.4	
15	NOV 1 82	7:00	90	No	3.9	0	-5	N	895	M	14	11.9	6.0	
16	NOV 1 82	7:25	90	No	3.6	0	-5	N	826	M	15	10.4	5.8	
17	NOV 7 82	13:00	20	No	1.1	0	63	U	60	C	22	0.023	0.47	
18	NOV 8 82	16:00	100	No	1.4	-5	5	N	321	C	22	0.022	0.22	
19	NOV 9 82	1:00	100	No	1.1	-14	-3	N	252	C	22	0.014	0.39	
20	NOV 14 82	20:25	0	Yes	3.9	2	-27	S	296	M	13	8.2	12.2	
21	NOV 14 82	22:05	10	Yes	1.7	-4	-25	S	78	M	15	7.3	90.8	
22	NOV 14 82	23:45	0	Yes	2.2	-4	-27	S	90	M	15	8.8	61.8	
23	NOV 15 82	3:15	10	Yes	3.9	0	-25	S	313	M	17	9.7	8.9	
24	NOV 15 82	8:00	30	Yes	3.1	-2	-20	S	197	L	21	1.5	7.1	
25	NOV 15 82	13:00	40	Yes	2.2	3	-17	S	90	C	22	1.6	25.9	
26	NOV 15 82	20:05	0	No	1.9	-5	-27	S	83	M	17	7.0	72.3	
27	NOV 15 82	23:00	0	No	0.8	-8	-27	S	49	M	15	8.5	54.1	
28	NOV 17 82	13:25	100	No	1.7	-8	17	U	208	M	8	4.8	13.2	
29	NOV 17 82	21:30	100	No	1.7	-8	-3	N	390	M	8	7.9	2.1	
30	NOV 18 82	20:00	100	Yes	1.9	-15	-3	N	436	M	8	10.9	1.2	
31	NOV 19 82	21:46	25	Yes	1.7	-20	-21	S	78	M	14	13.4	86.2	
32	NOV 20 82	19:30	0	Yes	2.8	-23	-27	S	104	M	13	14.0	43.2	
33	NOV 21 82	3:00	0	Yes	2.8	-25	-27	S	104	L	21	1.7	15.6	
34	NOV 21 82	5:41	0	Yes	2.8	-25	-27	S	104	M	22	8.8	27.3	
35	NOV 21 82	7:33	10	Yes	2.5	-25	-25	S	97	M	16	11.0	43.9	
36	NOV 21 82	8:37	10	Yes	2.2	-25	-25	S	90	M	19	14.6	48.3	
37	NOV 22 82	7:35	45	Yes	3.1	-11	-16	S	230	M	18	11.0	12.9	
38	NOV 22 82	7:52	65	Yes	3.1	-11	-11	S	283	M	18	10.3	11.4	
39	NOV 22 82	8:20	65	Yes	4.4	-10	-11	N	1009	M	19	9.7	5.5	
40	NOV 22 82	11:00	70	Yes	3.6	-10	-10	N	826	L	21	4.0	2.9	
41	NOV 23 82	17:30	40	Yes	0.8	-6	-17	S	49	M	22	8.5	80.6	
42	DEC 2 82	16:00	100	Yes	2.5	-6	-3	N	574	L	21	0.044	0.02	
43	DEC 2 82	17:00	100	Yes	1.9	-7	-3	N	436	C	22	0.029	0.08	
44	DEC 4 82	15:00	20	Yes	2.5	-2	-22	S	97	L	21	0.009	0.03	
45	DEC 5 82	13:00	70	Yes	1.7	-6	-10	S	78	L	21	0.020	0.00	
46	SEP 25 84	4:56	100	No	2.8	0	-3	N	436	M	0.3	3.5	2.9	
47	SEP 28 84	5:00	0	No	0.8	0	-27	S	25	G	18	0.018	0.80	
48	SEP 28 84	9:00	0	No	0.8	0	73	U	82	W	11	0.009	0.00	
49	DEC 13 85	8:30	60	Yes	0.7	-20	-13	S	31	M	3.5	0.7	28.3	
50	DEC 13 85	16:15	100	Yes	0.7	-20	-3	N	216	M	1.4	4.0	4.0	

Observations 1 to 45: Lodgepole
 Observations 46 to 48: Claresholm
 Observations 49 to 50: Rainbow Lake

U = Unstable Atmospheric Conditions
 N = Neutral Atmospheric Conditions
 S = Stable Atmospheric Conditions

L = Lodgepole Stationary Monitor
 C = Cynthia Stationary Monitor
 M = Mobile Monitor
 G = Granum Stationary Monitor
 W = Woodhouse Stationary Monitor

During the blowout, five stationary and five mobile air monitoring units were brought into the area to measure H_2S concentrations. The stationary units recorded hourly average values whereas the mobile units recorded peak values. The peak values represent an averaging period corresponding to the time constant of the instrumentation and sampling line. For the type of analyzers used, the peak values are assumed to be representative of a three minute averaging period.

Table 5.37 summarizes the maximum H_2S concentrations observed at the stationary units. In general, the observed values are relatively small (when compared to the Lodgepole blowout). The reports summarizing the mobile unit observations do not give exact locations of the monitoring sites, and as a consequence these observations cannot be used for model validation. The only mobile H_2S observation which could be correlated with a specific location is the value of 3.5 ppm observed 300 m to the south of the well at 04:56 on September 25.

The nearest Atmospheric Environment weather stations to the blowout site are Calgary International Airport (125 km north-northwest) and Lethbridge (70 km southeast). Additional wind data are available from the stationary ambient air monitors. Cloud cover and snow cover data were obtained from AES hourly data records for Lethbridge. Table 5.31 summarizes the meteorological data and the preprocessor predictions for surface heat flux (H_o), stability and mixing height (Z_i). The surface roughness length was estimated from the nature of the terrain surrounding the blowout site: for Claresholm (flat treeless terrain) Z_o was assumed to be 0.1 m.

5.8.3 Rainbow Lake Well Blowout

The Canterra and Mobile Rainbow well is located about 20 km southwest of the town of Rainbow Lake amid relatively flat forested terrain. The well was drilled in 1967 and was only recently completed. It was during the well completion and production testing phase that a failure occurred.

The uncontrolled release of gas began at 22:30 on December 9, 1985 and ended at 14:00 on December 14, 1985. A service rig, which was in place over the well head until 14:00 on December 13, 1985, deflected a portion of the vertically directed jet. After the service rig was moved 35 m from the well head, the vertical jet was not deflected. During the entire period the well remained unignited. Well blowout parameters are summarized in Table 5.36.

During the release period, three mobile air monitoring units were in operation. All monitoring data are summarized in reports which were prepared by the representative contractors. These reports, however, are of limited use due to ambiguities and inconsistencies in the data. That is, the observed H_2S concentration could not be correlated with a specific location over a known averaging period. During the blowout, a Canterra environment staff member directed one of the mobile units to obtain cross wind H_2S concentrations. These results are summarized in Table 5.31. The values presented in the table represent one to three minutes averaging periods. For model comparison purposes, however, a three minute averaging period is assumed.

The wind values given in Table 5.37 are based on the limited on-site information. Cloud cover and snow cover data were obtained from AES hourly data records for High Level. The table also provides the meteorological preprocessor predictions for surface heat flux

(H_o), stability and mixing height (Z_i). The surface roughness length was estimated from the nature of the terrain surrounding the blowout site: for Rainbow Lake (flat forested terrain) Z_o was assumed to be 0.5 m.

5.8.4 Model Predictions

Figure 5.64 compares model predictions with the observations selected in the previous section. The mobile H_2S observations have been normalized to a three minute average while those from stationary monitors have been normalized to a one hour averaging period using the power law relationship. Stationary SO_2 observations were normalized from a one hour average to a three hour average.

The diagonal lines on the figure represent the perfect 1:1 correlation (perfect agreement) and the "factor of two" envelope. The following is noted:

- Predicted values are scattered both above and below the 1:1 line. One is in perfect agreement with the observed value, 37 predicted values are above the 1:1 line (overprediction) and 12 predicted values are below the 1:1 line (underprediction).
- 14 predicted values are within a factor of two of the observed values. 31 predicted values are a factor of two or greater than the observed values and 5 predicted values are a factor of two or less than the observed values.
- The maximum observed value for the Lodgepole data is 15 ppm. The maximum predicted value for the Lodgepole data is 91 ppm.

Due to the previously discussed limitations with the input data, the calculation of formal correlation statistics was not warranted. In conclusion, the model appears (on the basis of limited data) to significantly overpredict.

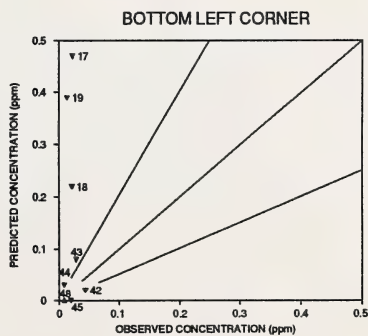
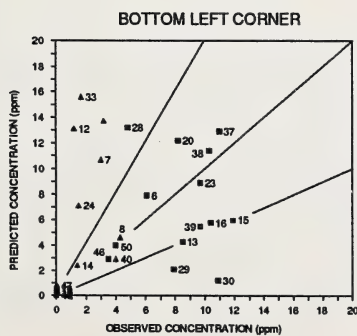
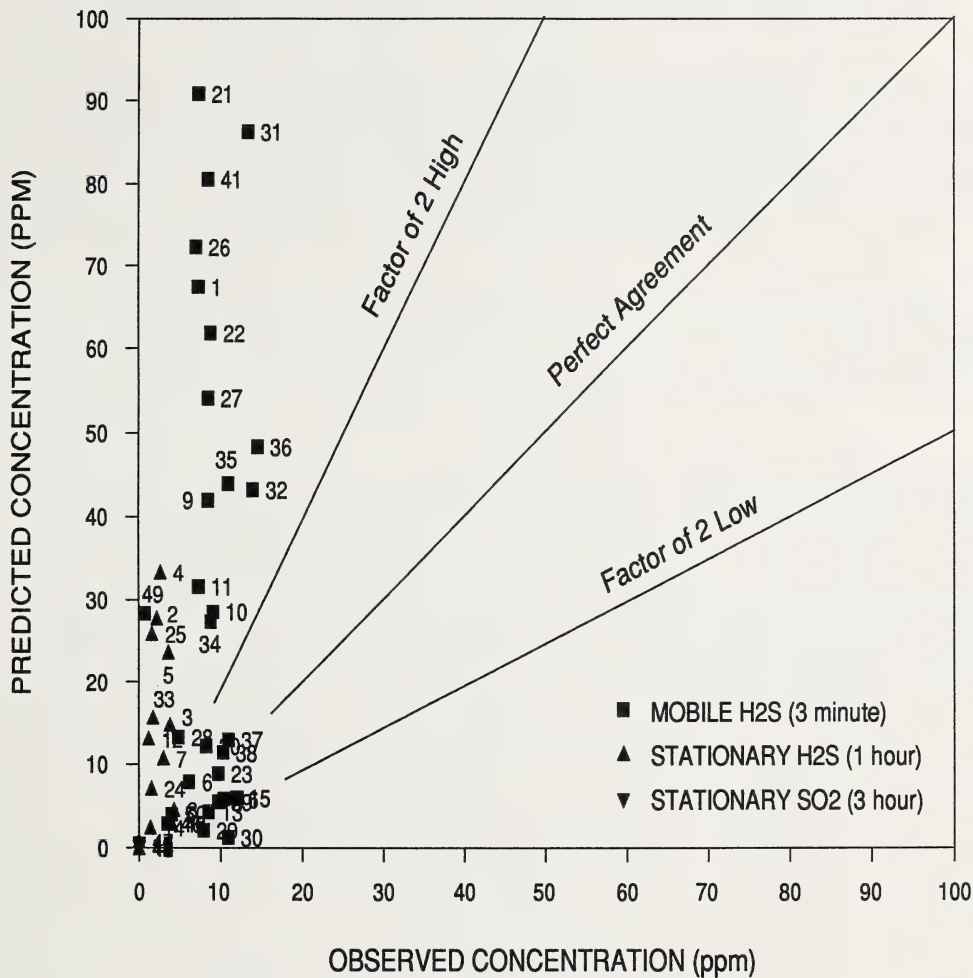


Figure 5.64

Predicted H₂S and SO₂ Concentrations for Selected Well Blowout Observations.

6 DISCUSSION, RECOMMENDATIONS AND CONCLUSIONS

A model for estimating downwind concentration and consequences from uncontrolled sour gas well and pipeline releases has been developed. During the development of the model, an attempt was made to use available *application* oriented submodels where possible. That is, the project objective was viewed as the development of an *applied* model and not viewed specifically as an exercise to integrate and unify the physics of jet expansion, plume rise and plume dispersion processes with detrimental effects modelling.

The model presented in this report has been computer coded and is referred to as "GASCON2" (Gas CONcentration and CONsequences). GASCON2 can be used by land developers, municipal planners, regulatory agencies and industry to estimate potential exposure zones and risk associated with sour gas facilities. This will aid in regional development and emergency response planning purposes.

The size of the potential hazard zone depends on user specified concentration (H_2S or SO_2) criteria. The individual risk, calculated for a given release event, consists of estimates of the probability of a lethal toxic load occurring at several locations downwind of the release point. The societal risk, again for a given event, consists of an estimate of the potential number of human fatalities due to the release. The magnitude of the risk estimates provided by GASCON2 is dependent on user specified probit parameters (giving the lethality of H_2S to humans) and the population density (given the potential number of people exposed to H_2S), in addition to all other user specified inputs. Consequence estimates are based solely on H_2S lethality in humans due to H_2S inhalation.

The following have not been incorporated in GASCON2:

- Hazards other than H_2S inhalation: thermal radiation, explosions.
- Sub-lethal effects due to H_2S inhalation.
- Risk reduction due to indoor exposure to H_2S .

GASCON2 is capable of providing estimates of risk to sensitive sub-populations and risk due to SO_2 inhalation, although it has not yet been applied to these situations. The former requires different sets of input probit parameters for each sub-population (eg. elderly people, asthmatics, etc.), which the published data presently cannot support. The latter requires a different set of input probit parameters for SO_2 toxicity which, in the context of the results for various ignited sour gas release scenarios reported, was deemed not necessary due to the clearly sub-lethal magnitude of estimated SO_2 concentrations.

6.1 Model Features

The methods presented in this report and incorporated into the modelling framework (which consists of the meteorological preprocessor as well as the GASCON2 model) contain a number of features which are relatively new to the estimation of concentration and consequences from uncontrolled sour gas releases. These features include:

Meteorological Preprocessor

- The development of a meteorological preprocessor to maximize the utility of conventional meteorological data for dispersion modelling purposes.
- The provision for a continuous range of planetary boundary layer variables within three major stability regimes instead of the frequently used six discrete Pasquill classes.
- Convective scaling (the use of W^* and Z_i) to define turbulence in unstable regimes.
- Surface-layer similarity scaling (the use of L and U^*) to define turbulence in the stable and neutral stability regimes.
- The existence of minimum or "residual" turbulence for low wind speed, stable regimes which define turbulence for wind speeds as low as 1 m/s.

Jet Expansion

- The incorporation of the jet expansion zone to account for the initial rise and dilution of high velocity jets.
- The development of a combustion module to account for the potential ignition of sour gas resulting in SO_2 production.

Plume Rise

- The adaptation of the integral plume rise approach to uncontrolled releases.
- The definition of additional plume rise termination criteria for the integral plume rise approach.
- The ability to estimate the rise of non-vertical momentum jets.
- The ability to estimate the rise of momentum jets directed into the wind.
- The incorporation of ground effects for horizontally released plumes.

Passive Dispersion

- The ability to estimate concentrations from transient as well as steady state releases.
- A plume penetration submodel which allows for the partial penetration of a plume into the free atmosphere above the mixing layer.
- The plume spreads for unstable and stable regimes are allowed to vary continuously according to the turbulence parameters obtained from the meteorological preprocessor.
- A minimum effective turbulence level for stable regimes where turbulence has a strong height dependence.

Consequences

- A fluctuating load model to account for turbulence-driven concentration fluctuation in the atmosphere. To the authors' knowledge, this is the first model to use a distribution function for the toxic load as defined in this report.
- A probit model for estimating the lethal effect of H₂S exposure to humans. The probit model, through the use of the toxic load concept, is able to give lethality estimates accounting for both concentration level and exposure time. The use of probit methods in risk assessment is a relatively recent development.
- Determination of probability of receiving a lethal toxic load of H₂S downwind of a release by combining the above concepts. This can be thought of as the individual risk for a given event.
- Estimation of potential fatalities (societal risk) assuming people are present and outdoors.

The integration of the submodels presented in this report is unique and the modelling system developed represents a comprehensive, model which can be applied to a wide range of uncontrolled release scenarios and meteorological conditions.

6.2 General Model Results

During the model sensitivity analyses (Section 5), GASCON2 was used to estimate ground level H_2S and SO_2 concentrations and consequences due to H_2S for a wide range of release and meteorological scenarios. While a wide range of scenarios was considered, it is no doubt possible to conceptualize additional scenarios not addressed specifically in the sensitivity analyses section. For this reason, the following general results from the model should be viewed as preliminary:

Well Blowouts

- Horizontal jet releases produce the largest H_2S concentrations and probabilities of lethality.
- Downwind jet releases produce larger H_2S concentrations than upwind jet releases.
- Vertical jet releases produce low H_2S concentrations due to higher plume rise.
- Larger H_2S concentrations and probabilities of lethality generally result from larger release rates.

Pipeline Ruptures

- Predicted H_2S concentrations and probabilities of lethality do not appear to be sensitive to the location of the break in a pipeline segment (for long ruptures).
- The largest H_2S concentrations and probabilities of lethality are predicted to result from the larger diameter, longer length pipelines.
- Downwind jet releases result in the largest predicted H_2S concentrations and probabilities of lethality.
- Vertical jet releases result in the smallest predicted H_2S concentrations.
- Increased delay times for the ESD valves to isolate the pipeline segment result in larger predicted concentrations and probabilities of lethality.
- Full ruptures (100% of hole area) result in the highest concentrations but a partial rupture of 50% results in the highest probability of lethality due to the increase in exposure time.

Meteorology

- Larger H_2S concentrations and probabilities of lethality are predicted for smaller values of surface roughness.
- Maximum SO_2 concentrations are not sensitive to surface roughness but the enhanced turbulence associated with larger surface roughness moves the peak nearer to the well.
- Predicted concentrations are relatively insensitive to ambient temperatures.
- The largest predicted concentrations for horizontal releases occur under low wind speed, stable conditions (for H_2S : 1 m/s and for SO_2 : 5 m/s).
- For neutral and unstable conditions, the highest predicted concentrations occur relatively close to the source and are associated with moderate to high wind speeds (3 to 15 m/s).

- Probabilities of lethality for neutral and unstable conditions were considerably less than for stable conditions.

In summary, the largest hazard zones and potential fatalities for unignited releases are associated with low wind, stable atmospheric conditions. For ignited release, the largest hazard zones are associated with moderate wind speed stable conditions.

6.3 Recommendations for Future Work

The development of GASCON2 has had the benefit of the Field Measurement Program (Volumes 1-4, ERCB (1990)) to verify the passive dispersion module. Since the time of the original release in 1987 (Alp *et al.* 1987), the physics and code have been thoroughly reviewed and revised where required. As of this release, not all of the recommendations that came out of the Field Measurement Program model evaluation (Volume 4) have been incorporated into the model. The major recommendations from Volume 4 were to:

- Revise the meteorological preprocessor criteria of using the surface heat flux alone to determine the stability condition. Estimated turbulence levels should also be reviewed.
- Review the formulations for crosswind plume spread and adjust to match observations.

In addition, there are areas where recommendations for future work can be made to increase the level of confidence in the model predictions. These recommendations, without regard to priority, are as follows:

- Based on the location of sour gas reserves in Alberta, extend the model capabilities to address complex terrain conditions. Conduct field studies to evaluate the effect of complex terrain on turbulent boundary layer parameters.
- Collect concurrent well source data, meteorological data, plume height data and concentration data associated with future uncontrolled well releases.
- Undertake further theoretical investigations followed by a field study to estimate the effective mass release rate. The field experiments would also supply much needed data on diffusion in the direction of the wind.
- Review criteria for ground versus elevated plumes.
- Verify the final plume rise for horizontal releases predicted by the integral plume rise module. This may require a field experiment as very few published observations are in the scientific literature.
- Undertake further theoretical investigations and comparisons with experimental data on the fluctuating load distribution.
- Extend the fluctuating load model to include indoor concentrations and consequences.

The ignition of the plume has been thought to mitigate undesirable health effects associated with an uncontrolled well blowout. To determine the relative effects of SO₂ versus H₂S emissions (ignition versus non-ignition), it is further recommended that:

- The selection of critical concentration values for both H₂S and SO₂ be reviewed keeping in mind the purpose of the critical value and the time period over which the concentration values are averaged.

6.4 Conclusions

The GASCON2 model incorporates our current understanding of the physics to produce an application oriented model which can be used to estimate concentrations and consequences which result from uncontrolled sour gas releases with more confidence than previously available models. It represents an advance over previous models used to assess the hazards associated with sour gas in that it incorporates the important influences of downwind concentration and exposure time to estimate the lethal potential. The model can be used as a tool to help ensure that public safety concerns are properly addressed in the vicinity of sour gas developments.

The general results of model runs presented in this report indicate that the H₂S concentrations are sensitive to the release angle and to the volume of the gas released. On this basis, the following can reduce the H₂S concentrations resulting from an uncontrolled release:

- For well blowouts, ensure that the release is directed vertically and not horizontally. This may be accomplished by providing barriers to redirect a horizontal release to a vertical flow.
- Install Emergency Shut Down (ESD) valves along a pipeline to decrease the volume of gas released to the atmosphere in the event of a pipeline rupture. Although the potential exposure zone may decrease with the installation of additional ESD valves, the risk associated with the pipeline may increase due to the increased number of exposed pipeline sections associated with the ESD valves.
- Avoid the use of large diameter pipelines close to population centers. Preliminary results seem to indicate that it may be beneficial to use a multiplicity of smaller diameter pipelines which together can transport the same flow rate of sour gas as the large diameter pipeline.
- Ignite the plume to convert H₂S to SO₂, the increased plume rise due to combustion will result in SO₂ concentrations which are smaller in magnitude than the unignited H₂S concentrations.

These conclusions are somewhat intuitive and can be reached without the use of a model. GASCON2, however, can quantify the magnitude of the benefit (in terms of the reduction in ground-level concentration and potential exposure zone size) of implementing various control strategies.

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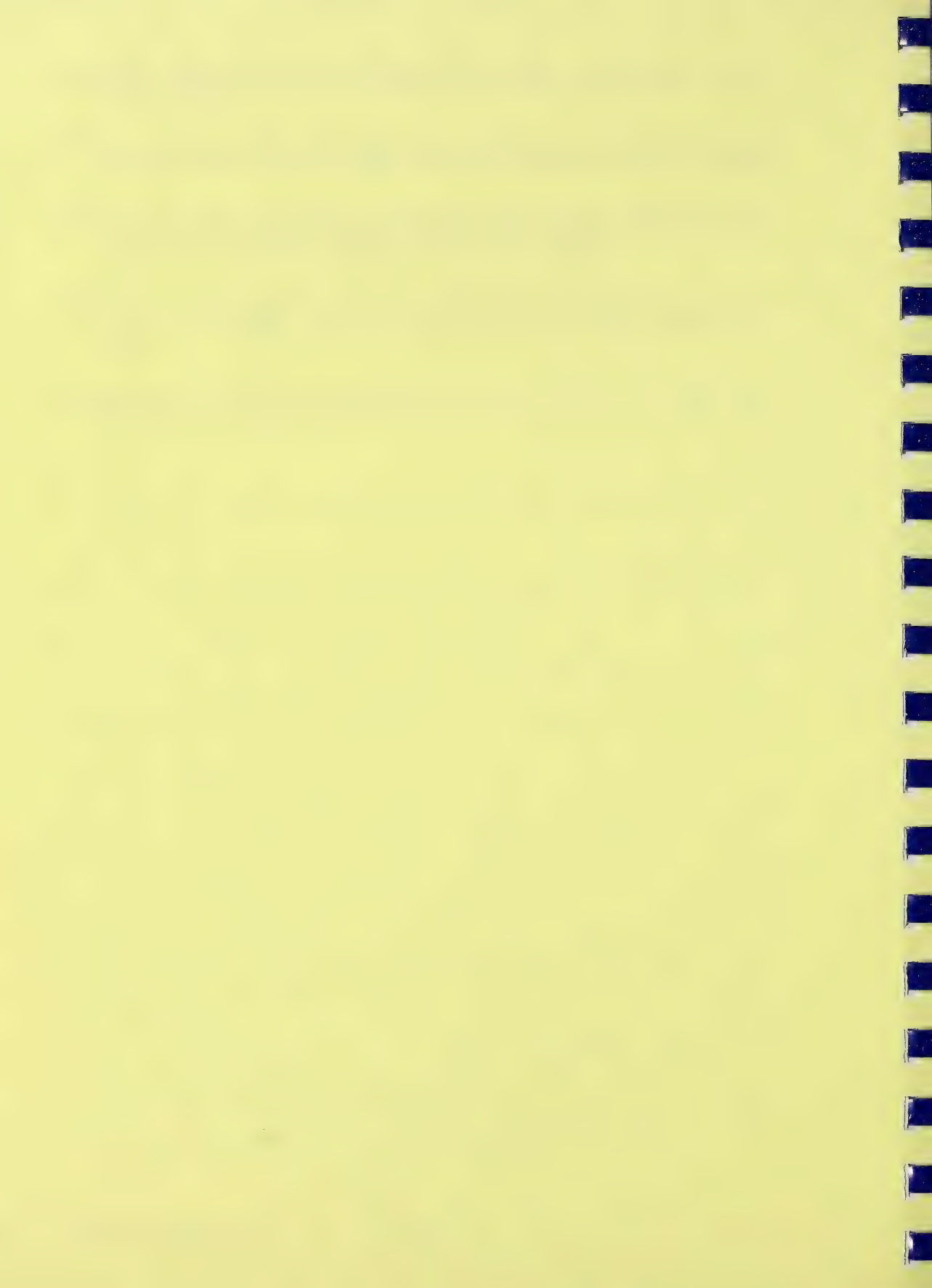
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8 SYMBOL GLOSSARY

Symbol	Description	Section
A_C	area of the jet at "C" plane (m^2)	4.2.5
A_D	area of the jet at "D" plane (m^2)	4.2.3
A_E	cross sectional area of rupture (m^2)	4.1.2
A_{EFF}	effective surface area between "Q" and "S" planes (m^2)	4.2.4
A_P	cross sectional area of pipe (m^2)	4.1.2
A_Q	area of the jet at "Q" plane (m^2)	4.2.2
A_S	area of the jet at "S" plane (m^2)	4.2.4
a	mass fraction CH_4 in sour gas	4.2.5
b	mass fraction H_2S in sour gas	4.2.5
b_I	strength of the inversion (m/s^2)	4.5.1
C	cloud cover in percent	3.1
C_D	drag coefficient	4.2.3
C_M	added mass factor to account for apparent additional mass of plume	4.3.1
C_F	skin friction coefficient of plume impinging on ground	4.3.1
C_L	lean flammability limit of combined CH_4 - H_2S stream, fraction by volume	4.2.5
$C_{L(CH_4)}$	CH_4 concentration at the lean flammability limit, fraction by volume (0.05)	4.2.5
$C_{L(H_2S)}$	H_2S concentration at the lean flammability limit, fraction by volume (0.042)	4.2.5
C_O	speed of sound in pipeline gas before rupture (m/s)	4.1.2
C_P	specific heat at constant pressure ($J/(kg\ K)$)	4.2.1
C_{PA}	specific heat of air at constant pressure ($J/(kg\ K)$)	3.1.2
C_{PC}	specific heat at constant pressure of combusted gas-air mixture ($J/(kg\ K)$)	4.2.5
C_{PCO_2}	specific heat at constant pressure of CO_2 ($J/(kg\ K)$)	4.2.5
C_{PD}	specific heat at constant pressure of the gas at "D" plane ($J/(kg\ K)$)	4.2.3
C_{PE}	specific heat at constant pressure of the gas at "E" plane ($J/(kg\ K)$)	4.2.1
C_{PH_2O}	specific heat at constant pressure of H_2O ($J/(kg\ K)$)	4.2.5
C_{PI}	specific heat at constant pressure of gas stream "I" ($J/(kg\ K)$)	Table 4.1

C_{PN_2}	specific heat at constant pressure of N_2 (J/(kg K))	4.2.5
C_{PO_2}	specific heat at constant pressure of O_2 (J/(kg K))	4.2.5
C_{PQ}	specific heat at constant pressure of the gas at "Q" plane (J/(kg K))	4.2.2
C_{PS}	specific heat at constant pressure of the gas-air mixture at "S" plane (J/(kg K))	4.2.4
C_{PSO_2}	specific heat at constant pressure of SO_2 (J/(kg K))	4.2.5
C_Q	sonic velocity at the "Q" plane	4.2.2
C_{VI}	specific heat at constant volume (J/(kg K))	Table 4.1
c	concentration of scalar species (e.g., H_2S) in the plume (kg/m ³)	4.3.1
D	Julian day of the year (1 to 365)	Table 3.1
$D(x,y)$	population density (people/m ²)	4.7.2
d	pipeline line diameter (m)	4.1.2
dT_A/dZ	vertical temperature gradient in the atmosphere	4.3.1
erf	mathematical error function	4.6
$erfc$	compliment of mathematical error function	4.4
F	pipeline friction factor	4.1.2
$F(L)dL$	toxic load probability density function	4.6.3
F_B	buoyancy flux (m ⁴ /s ³)	Table 4.4
F_M	momentum flux (m ⁴ /s ²)	Table 4.4
F_{RC}	Froude number with combustion	4.2.4
f	fraction of the plume remaining in the mixed layer	4.5.1
f_A	factor to account for plume cross-sectional area reduction due to ground impingement	4.3.1
f_C	Coriolis parameter	3.1.4
f_{CY}	dimensionless correction factor to force the Weil and Brower σ_Y values to equal the Briggs (1974) σ_Y values at large distances	4.5.4
f_{CZ}	dimensionless correction factor to force the Weil and Brower σ_Z values to equal the Briggs (1974) σ_Z values at large distances	4.5.4
f_E	factor to account for plume circumferential area reduction due to ground impingement	4.3.1
f_{EDGE}	entrainment value to define f_{MIN}	4.5.1
f_{MIN}	minimum value of f	4.5.1
f_R	fraction of heat produced by combustion which is lost by radiation	4.2.5

$f_Y(x)$	dimensionless function which relates cross wind velocity fluctuations to cross wind plume spread	4.5.4
$f_Z(x)$	dimensionless function which relates vertical wind velocity fluctuations to vertical plume spread	4.5.4
g	acceleration of gravity	3.1.3
H_L	long wave radiation losses from the surface (W/m ²)	3.1.1
H_O	surface heat flux (W/m ²)	3.1
Δh	Briggs' final plume rise (m)	4.3.3
Δh_B	final buoyancy rise (m)	4.3.3
$(\Delta h_B)_N$	final buoyancy rise in neutral conditions (m)	4.3.3
$(\Delta h_B)_S$	final buoyancy rise in stable conditions (m)	4.3.3
$(\Delta h_B)_U$	final buoyancy rise in unstable conditions (m)	4.3.3
Δh_M	final momentum rise (m)	4.3.3
Δh_{SC}	stable plume rise relationship applicable to near calm conditions (m)	4.3.3
Δh_1	"sum of cubes" final rise for non-calm conditions (m)	4.3.3
Δh_2	"sum of cubes" final rise for near calm conditions (m)	4.3.3
i_p	fluctuation intensity	4.7.2
I_1	first term in analytical expression for the effective mass release rate	Table 4.6
I_2	second term in analytical expression for the effective mass release rate	Table 4.6
I_3	third term in analytical expression for the effective mass release rate	Table 4.6
k	von Karman constant	3.1.3
k_1	probit parameter	4.6.1
k_2	probit parameter	4.6.1
k_D	ratio of specific heats for the pipeline gas (C_p/C_v) at "D" plane	4.2.3
k_E	ratio of specific heats for the pipeline gas (C_p/C_v)	4.1.2
k_Q	ratio of specific heats for the pipeline gas (C_p/C_v) at "Q" plane	4.2.2
k_S	ratio of specific heats for the gas-air mixture (C_p/C_v) at "S" plane	4.2.4
L	Monin-Obukhov length (m)	2.3.2
L	toxic load (ppm ⁿ min)	4.6.1

L_C	length between "S" and "C" planes (m)	Figure 4.2
L_D	jet length between "Q" and "D" planes (m)	Figure 4.2
L_I	independent Monin-Obukhov length from Table 3.5	Table 3.5
L_O	longitude of site (degrees)	Table 3.1
L_M	median toxic load	4.7.2
L_Q	jet length between "E" and "Q" planes (m)	Figure 4.2
L_S	jet length between "D" and "S" planes (m)	Figure 4.2
L_{ST}	time zone standard longitude (degrees)	Table 3.1
L_T	latitude of site (degrees)	Table 3.1
L_{50}	toxic load which causes 50% mortality in population	4.6.1
$\bar{L}$	mean toxic load	4.7.2
l	pipeline length (m)	4.1.2
l_{EFF}	effective pipeline length to allow for the extra gas released during the time taken for the ESD valves to fully close	4.1.2
M_S	Mach number at "S" plane	4.2.3
M_T	total mass to be released (kg)	4.1.2
M_{WA}	molecular weight of air (28.95 kg/kmole)	4.2.4
M_{WC}	molecular weight of combusted gas-air mixture at "C" plane (kg/kmole)	4.2.5
M_{WD}	molecular weight of the gas at "D" plane (kg/kmole)	4.2.3
M_{WCO_2}	molecular weight of CO ₂ (44 kg/kmole)	4.2.5
M_{WE}	molecular weight of the discharging gas at "E" plane (kg/kmole)	4.2.1
M_{WH_2O}	molecular weight of H ₂ O (18 kg/kmole)	4.2.5
M_{WI}	molecular weight of gas stream "I" (kg/kmole)	Table 4.1
M_{WN_2}	molecular weight of N ₂ (28 kg/kmole)	4.2.5
M_{WO_2}	molecular weight of O ₂ (32 kg/kmole)	4.2.5
M_{WQ}	molecular weight of the gas at "Q" plane (kg/kmole)	4.2.2
M_{WS}	molecular weight of the gas-air mixture at "S" plane (kg/kmole)	4.2.4
M_{WSO_2}	molecular weight of SO ₂ (64 kg/kmole)	4.2.5
$\dot{m}_A$	mass flow of air entrained between "Q" plane and "S" plane (kg/s)	4.2.4
$(\dot{m}_A)_C$	mass flow of air at "C" plane (kg/s)	4.2.4

$\dot{m}_{AC}$	mass flow of air entrained between "S" plane and "C" plane (kg/s)	4.2.5
$\dot{m}_C$	mass flow of combusted gas-air mixture at "C" plane (kg/s)	4.2.5
$(\dot{m}_C)_{CO_2}$	mass flow of CO ₂ at "C" plane (kg/s)	4.2.5
$(\dot{m}_C)_{H_2O}$	mass flow of H ₂ O at "C" plane (kg/s)	4.2.5
$(\dot{m}_C)_{N_2}$	mass flow of N ₂ at "C" plane (kg/s)	4.2.5
$(\dot{m}_C)_{O_2}$	mass flow of O ₂ at "C" plane (kg/s)	4.2.5
$(\dot{m}_C)_{SO_2}$	mass flow of SO ₂ at "C" plane (kg/s)	4.2.5
$MAX[a,b]$	function which determines maximum of a and b	4.3.2
$MIN[a,b]$	function which determines minimum of a and b	4.1.3
$\dot{m}_E$	mass flow rate of gas at "E" plane (kg/s)	4.1.1
$\dot{m}_D$	mass flow of gas at the "D" plane	4.2.3
$\dot{m}_E(t)$	mass release rate at time t (kg/s)	4.1.3
$\dot{m}_E(\tau)$	mass release rate at time τ (kg/s)	4.4
$\dot{m}_{EFF}(x_1, t)$	effective mass flux at distance x_1 which accounts for along wind diffusion (kg/s)	4.4
$\dot{m}_{E,S}$	steady state mass release rate portion	4.1.3
$\dot{m}_{E,T}(t)$	transient mass release rate portion at time t	4.1.3
$\dot{m}_O$	initial gas release rate at time $t=0$ s (kg/s)	4.1.2
$\dot{m}_p$	mass flow rate of the given plume component (H ₂ S or SO ₂) in the release (kg/s)	4.5.4
$\dot{m}_Q$	mass flow of gas at the "Q" plane	4.2.2
$\dot{m}_S$	mass flow of gas-air mixture through the "S" plane (kg/s)	4.2.4
n	probit parameter	4.6.1
n	velocity profile power law exponent, used to estimate σ_x	4.4
N_F	potential fatalities	4.7.2
P	buoyancy parameter used to determine fraction of the plume remaining in the mixed layer for unstable conditions	4.5.1
P_{AO}	surface pressure (Pa)	3.1

P_D	pressure of the gas at "D" plane (Pa)	4.2.3
P_E	pressure of the gas at "E" plane (Pa)	4.2.1
$P_E(x)$	probability of a critical concentration level being exceeded	4.6.8
P_O	gas pressure in pipeline before rupture (P_A)	4.1.2
P_Q	pressure of the gas at "Q" plane (Pa)	4.2.2
P_S	pressure of the gas-air mixture at "S" plane (kPa)	4.2.3
P_Y	power used to estimate Pasquill-Smith cross wind plume spread	Table 5.35
P_Z	power used to estimate Pasquill-Smith vertical plume spread	Table 5.35
$P(L)$	probability that the toxic load L is lethal	4.6.1
$P_L(x,y)$	probability of receiving a lethal toxic load at position (x,y)	4.7.2
$P_L(x,y)$	probability of the mean toxic load being lethal	4.7.2
p	wind speed power law exponent	Table 3.5
Q_H	heat produced by the combustion reaction (J/m^3)	4.2.5
Q_{HI}	heat of combustion of gas stream "I" (J/m^3)	Table 4.1
q	averaging time correction exponent, dependent upon atmospheric stability	4.5.2
$\bar{q}$	stability parameter for unstable conditions	3.1.3
$\bar{R}$	net short wave solar radiation (W/m^2)	3.1.1
R_A	gas constant for air (287 J/(kmole kg))	3.1.3
R_C	gas constant of the combusted gas-air mixture at "C" plane (J/(kg K))	4.2.5
R_D	particular gas constant at "D" plane (J/(kg K))	4.1.3
R_E	particular gas constant at "E" plane (J/(kg K))	4.1.1
R_I	particular gas constant for gas stream "I" (J/(kg K))	Table 4.1
R_Q	particular gas constant at "Q" plane (J/(kg K))	4.2.2
R_S	particular gas constant of the gas-air mixture at "S" plane (J/(kg K))	4.2.4
R_U	universal gas constant ($8314.4 \text{ J/(kmole K)}$)	Table 4.1
S	stability parameter used for estimating plume rise in stable conditions (s^{-2})	4.3.3
S_L	toxic load standard deviation	4.6.3
r	plume radius (m)	4.3.1
R_F	plume radius at the downwind distance X_F (m)	4.5.2
r_o	equivalent radius of jet at "S" plane	4.3.1
r_{ST}	radius of the stack (m)	Table 5.34
S_o	square of the Brunt-Vaisala frequency (s^{-2})	4.3.3
s	plume centerline coordinate (m)	4.3.1

T	plume temperature (K)	4.3.1
T_{AO}	ambient temperature (K)	4.3.1
$T_{AO(max)}$	maximum ambient temperature during the day (K)	3.1.2
$T_{AO(min)}$	minimum ambient temperature after sunrise (K)	3.1.2
$T_{AO}(t)$	ambient temperature at time t (K)	3.1.2
$\bar{T}_{AO}$	average temperature in the convective boundary layer (K)	3.1.3
T_C	temperature of the combusted gas-air mixture at "C" plane (K)	4.2.5
T_D	temperature of the gas at "D" plane (K)	4.2.3
T_E	temperature of the gas at "E" plane (K)	4.2.1
T_O	temperature of gas in pipeline before rupture (K)	4.1.2
T_Q	temperature of the gas at "Q" plane (K)	4.2.2
T_S	temperature of the gas-air mixture at "S" plane (K)	4.2.4
t	time	
t_1	averaging time (s)	4.5.2
t_2	averaging time (s)	4.5.2
t_{AVG}	averaging time (s)	Table 5.35
t_E	exposure time (min)	4.6.1
t_N	local standard noon time in decimal hours	Table 3.1
t_{RISE}	local sunrise time in decimal hours	Table 3.1
t_S	time at which the steady state mass release rate dominates in a continuous pipeline release (s)	4.1.3
t_{SET}	local sunset time in decimal hours	Table 3.1
U	ambient windspeed (varies with z) (m/s)	4.3.1
$\bar{U}$	mean transport wind speed of the plume (m/s)	4.4
$U(0.1Z_i)$	wind speed at one tenth of mixed layer height Z_i	4.5.4
$U(z)$	wind speed at height z (m/s)	4.4
U^*	surface friction velocity (m/s)	2.3.2
U_1	wind speed at height Z_1 (m)	3.1.6
U_2	wind speed at height Z_2 (m)	3.1.6
U_C	ambient wind speed at height of "C" plane (m/s)	4.2.4
U_D	ambient wind speed at height of "D" plane (m/s)	4.2.4
U_F	wind speed at height Z_F (m/s)	4.5.4
U_P	wind speed at plume height (m/s)	4.3.2
U_{REF}	wind speed at anemometer height (m/s)	2.3.4
U_S	ambient wind speed at height of "S" plane (m/s)	4.2.5
U_{ST}	wind speed at stack height (m/s)	Table 5.34

V	plume velocity (m/s)	4.3.1
$\dot{V}$	volume flow rate of sour gas (m ³ /d)	4.1.1
V_C	velocity of the combusted gas-air mixture at "C" plane (m/s)	4.2.5
V_D	velocity of the gas at "D" plane (m/s)	4.2.3
V_{CH_4}	volume fraction CH ₄ in the escaping gas	4.2.5
V_{CO_2}	volume fraction CO ₂ in the escaping gas	4.2.5
V_α	entrainment velocity, for parameterizing the amount of ambient air which is entrained into the plume (m/s)	4.3.1
V_E	velocity of the gas at "E" plane (m/s)	4.2.1
V_F	velocity of plume at Z_F (m/s)	4.5.4
V_F	relative velocity between the plume and the ground (m/s)	4.3.1
V_{EFF}	effective tangential velocity difference (m/s)	4.2.4
V_{H_2S}	volume fraction H ₂ S in the escaping gas	4.2.5
V_Q	velocity of the gas at "Q" plane (m/s)	4.2.2
V_R	relative velocity between the plume and the atmosphere (m/s)	4.3.1
V_S	velocity of the gas-air mixture at "S" plane (m/s)	4.2.3
V_{ST}	velocity of the effluent gas (m/s)	Table 5.34
V_{SZ}	vertical component of V_S (m/s)	Table 4.4
V_X	horizontal velocity component of plume (m/s)	4.3.1
V_Z	vertical velocity component of plume (m/s)	4.3.1
W^*	convective velocity scale (m/s)	2.3.2
X_S	distance from a virtual source (m)	Table 4.6
X_{SY}	distance from a virtual y-source (m)	Table 4.7
X_{SZ}	distance from a virtual z-source (m)	Table 4.7
X_{VY}	virtual distance to account for the spread of the plume in the cross wind direction (m)	Table 4.7
X_{VZ}	virtual distance to account for the spread of the plume in the vertical direction (m)	Table 4.7
X_V	virtual distance to account for the initial spread of the plume (m)	Table 4.6
X^*_{SY}	non-dimensional distance from a virtual y-source for surface plumes	4.5.5
X^*_{SZ}	non-dimensional distance from a virtual z-source for surface plumes	4.5.5
x	horizontal coordinate or downwind distance (m)	4.3.1

X_F	downwind distance from rupture point when integral plume rise model is terminated (m)	4.3.2
x_{REF}	reference distance	Table 5.29
x_S	virtual distance (m)	4.3.2
x_V	distance source for trajectory Equation 4.98	4.3.2
y	cross wind distance (m)	4.5.4
Y	probit function	4.6.1
$\bar{Z}$	mean height to which plume has dispersed (m)	4.5.5
$\bar{Z}_{AVG}$	average height used in the estimation of the wind speed power law exponent p (m)	Table 3.5
Z_C	elevation of "C" plane above the ground (m)	Figure 4.2
Z_D	elevation of "D" plane above the ground (m)	Figure 4.2
$\tilde{Z}_C$	pipeline gas compressibility prior to rupture	4.1.2
Z_E	elevation of "E" plane above the ground (m)	Figure 4.2
$\tilde{Z}_E$	gas compressibility at the exit	4.1.2
Z_F	plume elevation when the integral plume rise model is terminated (m)	4.3.2
Z_i	mixing height (m)	2.3.2
Z_M	height to estimate stability parameter for plume rise evaluation (m)	4.3.3
Z_O	surface roughness length (m)	3.1.3
Z_P	plume elevation (m)	4.3.2
Z_{PF}	final plume elevation above ground level or in the case of partial plume penetration, the height of the remaining portion of the plume in the mixed layer (m)	4.3.3
$Z_{PF,BRIGGS}$	Briggs' final plume elevation (m)	4.3.3
$Z_{PF,PEN}$	final elevation of the plume if plume penetration is predicted (m)	4.5.1
Z_Q	elevation of "Q" plane above the ground (m)	Figure 4.2
Z_R	function used to estimate σ_x (m)	4.4
Z_{REF}	anemometer height (m)	3.1.3
Z_S	elevation of "S" plane above the ground (m)	Figure 4.2
$Z_{PF,MAX}$	maximum elevation of plume (m)	4.3.2
Z_{SC}	plume elevation for near calm conditions (m)	4.3.3
Z_V	function used to estimate σ_x (m)	4.4
z	vertical coordinate (m)	4.3.1

Greek Symbol	Description	Section
α	entrainment constant	4.2.4
$\tilde{\alpha}$	reduction factor due to surface reflectivity	3.1.1
α_2	constant, dependent upon stability, used to estimate σ_x constant	4.4
β	entrainment constant	4.3.1
$\tilde{\beta}$	reduction factor due to cloud cover	3.1.1
Γ	inertial delay factor	4.1.2
γ	conditional plume fluctuation intensity	4.7.2
γ	minimum lapse rate after sunrise (K/m) ($\gamma = -dT/dz$)	3.1.2
γ_D	dry adiabatic lapse rate (0.0098 K/m)	3.1.2
δ	portion of plume above the ground (m)	4.3.1
δ	additional mass by ESD values as fraction of total mass	4.1.2
δ	solar declination (radian)	Table 3.1
δi	uncertainty in parameter i	5.6.3
ε	time constant in Equation 4.5 (s)	4.1.2
ζ	term used in Equation 3.31 and defined by Equation 3.32	Table 3.5
ζ_o	term used in Equation 3.31 and defined by Equation 3.32	Table 3.5
η	mass conservation factor	4.1.2
θ	potential temperature of plume (K)	4.3.1
θ_A	potential temperature of the atmosphere (varies with z depending upon stability) (K)	4.3.1
$\Delta\theta_i$	change in potential temperature across the depth of the inversion	4.5.1
$\partial\theta/\partial Z$	potential temperature gradient (K/m)	4.3.1
λ	angle of jet with horizontal (degrees)	4.2.3
λ_C	angle of combusted jet with horizontal (degrees)	4.2.5
ρ	density of plume (kg/m ³)	4.3.1
ρ_{AO}	ambient air density (varies with z) (kg/m ³)	3.1.2
ρ_C	density of the combusted gas-air mixture at "C" plane (kg/m ³)	4.2.4
ρ_D	density of the gas at "D" plane (kg/m ³)	4.2.3
ρ_E	density of the gas at "E" plane (kg/m ³)	4.2.1
ρ_{EO}	density of sour gas at standard conditions of 15 °C and 101.3 kPa	4.1.1
ρ_Q	density of the gas at "Q" plane (kg/m ³)	4.2.2
ρ_S	density of the gas-air mixture at "S" plane (kg/m ³)	4.2.4
σ_L	standard deviation of toxic load for frequency of mortality	4.6.1

σ_v	standard deviation of the cross wind speed fluctuations (m/s)	4.5.4
σ_w	standard deviation of the vertical wind speed fluctuations (m/s)	4.5.4
σ_{x_1}	standard deviation of the transient plume in the along wind direction at downwind distance x_1 (m)	4.4
σ_{y_t}	standard deviation of the plume in the cross wind direction averaged over t minutes (m)	4.5.4
σ_{y_1}	horizontal plume spread for averaging time t_1 (m)	4.5.2
σ_{y_2}	horizontal plume spread for averaging time t_2 (m)	4.5.2
σ_{YREF}	reference cross wind plume spread which depends upon boundary layer stability and roughness length (m)	Table 5.35
σ_z	standard deviation of the plume in the vertical direction (m)	4.5.4
σ_{ZREF}	reference vertical plume spread which depends upon boundary layer stability and roughness length (m)	Table 5.35
τ	lagged time after release used to calculate the transient mass release rate (s)	4.4
$\tilde{\tau}$	hour angle (radian)	Table 3.1
ϕ	plume angle with respect to the ground, defined in Equation 4.95	4.3.1
$\tilde{\phi}$	solar elevation angle above the horizon	3.1.1
$\overline{\chi}$	ensemble average concentration (kg/m ³)	4.7.2
χ_L	critical concentration level (kg/m ³)	4.7.2
χ_{MP}	maximum peak concentration accounting for fluctuation (kg/m ³)	4.7.2
$\chi_i(x,0,0)$	concentration of a given plume component (H ₂ S or SO ₂) at position (x,0,0) averaged over t minutes (kg/m ³)	4.5.2
$\chi_i(x,y,z)$	concentration of a given plume component (H ₂ S or SO ₂) at position (x,y,z) averaged over t minutes (kg/m ³)	4.5.2
Ψ	stability parameter for unstable conditions	3.1.3
Ω	earth's rotation rate (7.292•10 ⁻⁵ s ⁻¹)	3.1.4

Symbol**Chemical Symbols**

C ₁	methane
C ₂	ethane
C ₃	propane
C ₄	butanes
CH ₄	methane
CO ₂	carbon dioxide
H ₂ O	water
H ₂ S	hydrogen sulphide
N ₂	nitrogen
O ₂	oxygen
SO ₂	sulphur dioxide



APPENDIX A

PROBABILITY DENSITY FUNCTION FOR THE FLUCTUATING LOAD

Appendix A

The probability density function for the fluctuating load, introduced in Section 4.6, is;

$$F(L) = \frac{1}{\sqrt{2\pi}LS_L} \exp\left(\frac{-\ln^2\left(\frac{L}{L_M}\right)}{2S_L^2}\right) \quad (\text{A.1})$$

This log-normal distribution was derived by Wilson (1987), as an extension to earlier work (Wilson, 1986; Wilson and Simms, 1985). In this Appendix, a closed set of equations for the median load L_M and the standard deviation S_L is presented. For brevity, only a cursory discussion of issues related to concentration (and load) fluctuations is presented here; for more detailed discussion and for derivations of the equations presented in this Appendix, the reader is referred to Wilson (1986) and Wilson and Simms (1985).

From the properties of the log-normal distribution, one can show that the median load is related to the mean load by:

$$L_M = \bar{L} \exp\left(\frac{-S_L^2}{2}\right) \quad (\text{A.2})$$

Hence, specification of $\bar{L}$ and S_L is sufficient to determine $F(L)$. From Wilson (1986), the standard deviation of concentration fluctuations is:

$$S = [\ln(1 + i_p^2)] \quad (\text{A.3})$$

Where i_p is the conditional fluctuation intensity or plume intensity defined by:

$$i_p \equiv \frac{\sqrt{C_p'^2}}{\bar{C}_p} \quad (\text{A.4})$$

where $\bar{C}_p$ is the mean conditional concentration and C_p' is the conditional concentration fluctuation. The word "conditional" is taken to mean "when the toxic gas plume is overhead." All dispersion models predict $\bar{C}$, the average concentration, even when the plume is not overhead. The plume intermittency (γ) is defined as:

$$\gamma \equiv \frac{\bar{C}}{C_p}, \quad 0 \leq \gamma \leq 1 \quad (\text{A.5})$$

where γ is the fraction of time that the concentration is above zero.

The general definition of the toxic load is:

$$L \equiv \int_0^{t_e} C^n dt \quad (\text{A.6})$$

Where t_e is the exposure time in minutes and C is the predicted concentration (may be a function of time) averaged over the event time t_e . The constant n is one of the probit parameters discussed in Section 4.6. For steady gas releases, where C is not a function of time and the exposure time equals the event time:

$$L \equiv C^n t_e \quad (\text{A.7})$$

Because the toxic load L is essentially a higher moment of the concentration C , one can show that the standard deviation of toxic loads (S_L) is related to the standard deviation of concentrations (S) by:

$$\begin{aligned} S_L &= nS \\ &= n[\ln(1 + i_p^2)]^{1/2} \end{aligned} \quad (\text{A.8})$$

Hence, closure for equations (G.1) boils down to specifying i_p and $\bar{L}$.

Using the definition of the toxic load L , Equation (A.5) for $\overline{C_p}$, and the following relationship between $(\overline{C_p})^n$ and $\overline{C_p^n}$:

$$\frac{\overline{C_p^n}}{(\overline{C_p})^n} = (1 + i_p^2)^{\frac{n(n-1)}{2}} \quad (\text{A.9})$$

One can express the average toxic load ($\bar{L}$) as:

$$\begin{aligned} \bar{L} &= \int_0^{t_e} \gamma C_p^n dt \\ &= \int_0^{t_e} \gamma (\overline{C_p})^n dt \\ \bar{L} &= \int_0^{t_e} \left[\frac{(1 + i_p^2)^{\frac{n}{2}}}{\gamma} \right]^{n-1} (\overline{C_p})^n dt \end{aligned} \quad (\text{A.10})$$

Dispersion model predictions give $\bar{C}$, either as a constant in time (steady release) or as a function of time (transient release). Because $\bar{C}$ also is a function of downwind distance x and crosswind distance y , so then $\bar{C} = \bar{C}(x,y)$. Equation (G.10) implies that i_p and γ are the important parameters for ultimately determining L_M and S_L in Equation (G.1).

One can define a fluctuation intensity i which is not conditional, that is, one that is based on the concentration irrespective of whether the plume is overhead:

$$i \equiv \frac{\sqrt{\overline{C'^2}}}{\bar{C}} \quad (\text{A.11})$$

It is possible to find the relationship between i_p and i by noting:

$$C' = C - \bar{C} \quad \text{for } C \geq 0 \quad (\text{A.12})$$

and

$$C'_p = C - \bar{C}_p \quad \text{for } C > 0$$

From these two relations it is possible to show, by squaring and time means averaging, that:

$$\frac{\overline{(C')^2}}{(\bar{C})^2} = i^2 = \frac{\overline{C^2}}{(\bar{C})^2} - 1 \quad (\text{A.13})$$

and

$$\frac{\overline{(C'_p)^2}}{(\bar{C}_p)^2} = i_p^2 = \frac{\overline{C_p^2}}{(\bar{C}_p)^2} - 1$$

Combining these two relations:

$$\frac{i_p^2 + 1}{i^2 + 1} = \frac{(\bar{C})^2 \overline{C_p^2}}{(\bar{C}_p)^2 \overline{C^2}} = \gamma^2 \frac{\overline{C_p^2}}{\overline{C^2}} \quad (\text{A.14})$$

The conditional statistic $\overline{C_p^2}$ and the total statistic $\overline{C^2}$ are related by the intermittency γ ,

$$\overline{C^2} = \gamma \overline{C_p^2} \quad (\text{A.15})$$

Since γ is the fraction of time the plume is overhead. Hence, Equation (A.14) becomes:

$$\gamma = \frac{i_p^2 + 1}{i^2 + 1} \quad (\text{A.16})$$

Hence, if a closed set of equations for i_p and i can be specified, the probability density function $F(L)$ in Equation (A.1) will be determined.

Up to this point in this Appendix the relationships introduced for determining L_M and S_L in Equation (A.1) follow from properties of the log-normal distribution or from definitions. The closure equations for i_p and i follow from the semi-empirical analysis appearing in Wilson (1986) and Wilson and Simms (1985).

The starting point in the closure for i_p and i is the introduction of the fluctuation intensities $i_{p\infty}$ and i_{∞} , which are fluctuation intensities in the absence of a variance "sink" term at the ground from Wilson (1986):

$$i_{p\infty} = \frac{0.34\lambda}{\lambda^2 + (0.12)^2} \exp\left[\frac{-(z_p - h_v)^2}{4\sigma_z^2}\right] \quad (\text{A.17})$$

$$i_{\infty} = \frac{0.34\lambda}{\lambda^2 + \lambda_o^2} \exp\left[\frac{y^2}{4\sigma_y^2}\right] \exp\left[\frac{2z_p^2 - h_v^2}{4\sigma_z^2}\right] \quad (\text{A.18})$$

where λ is a non-dimensional parameter:

$$\lambda \equiv \frac{\sqrt{\sigma_y \sigma_z}}{z_i} \quad (\text{A.19})$$

and where y = crosswind distance (m)

z_p = plume height (m)

z_i = mixed layer height (m)

σ_y = 3-minute lateral plume standard deviation (m)

σ_z = 3-minute vertical plume standard deviation (m)

and

$$\lambda_o = \frac{0.12}{1 + 0.055 \frac{\Lambda}{2R}} \quad (\text{A.20})$$

with

$$\Lambda = 0.6z_p \exp \left[- \left(\frac{\sigma_z}{z_p} \right)^2 \right] \quad (\text{A.21})$$

R = plume (jet) radius at 1 second after the onset of the release (m) and
 h_v = fluctuation variance "source" height used in the Wilson (1986) model

$$h_v = [z_p^2 + 0.498\sigma_z^2]^{\frac{1}{2}} \quad (\text{A.22})$$

The relationship between i_∞ and i is presented in Wilson (1986) and can be simplified to read:

$$i = 0.316i_\infty \quad (\text{A.23})$$

where ground level ($z = 0$) has been assumed. The relationship between i_p and $i_{p\infty}$ is the same:

$$i_p = 0.316i_{p\infty} \quad (\text{A.24})$$

where again ground level ($z = 0$) has been assumed.

Equations A.17 to A.24 apply for event times t_E less times than or equal to 3 minutes. For event time t_E greater than 3 minutes, i_∞ (but from Equation A.23 not $i_{p\infty}$) must be adjusted for plume meandering to $i_{\infty t_E}$ by using $i_{\infty t_E}$.

$$\frac{1 + i_{\infty t_E}^2}{1 + i_\infty^2} = \frac{\sigma_{yt_E}}{\sigma_y} = \left(\frac{t_E}{3} \right)^2 \quad (\text{A.25})$$

It must be noted that all equations used to estimate the probability density functions are based on two important, simplifying assumptions:

- It is assumed that i_p is independent of the exposure time (t_e) over which the toxic load is integrated. In reality, i_p will decrease with exposure time as high frequency fluctuations are damped out. Neglecting this decrease will give higher peak loads.
- It is assumed that the exposure time t_e for toxic load is long enough that no zero values of toxic load will ever be observed, so $\gamma_L = 1.0$. This greatly simplifies the calculations, but will produce higher peak toxic loads.

The following equations form a closed set for the parameters L_M and S_L in Equation (A.1):

$$L_M = \bar{L} \exp\left(\frac{-S_L^2}{2}\right) \quad (\text{A.2})$$

$$S_L = n [\ln(1 + i_p^2)]^{1/2} \quad (\text{A.8})$$

$$\bar{L} = \int_0^{t_e} \left[\frac{(1 + i_p^2)^{\frac{n}{2}}}{\gamma} \right]^{n-1} (\bar{C})^n dt \quad (\text{A.10})$$

$$\gamma = \frac{i_p^2 + 1}{i^2 + 1} \quad (\text{A.16})$$

$$i_{p\infty} = \frac{0.34\lambda}{\lambda^2 + (0.12)^2} \exp\left[\frac{-(z_p - h_v)^2}{4\sigma_z^2}\right] \quad (\text{A.17})$$

$$i_{\infty} = \frac{0.34\lambda}{\lambda^2 + \lambda_o^2} \exp\left[\frac{y^2}{4\sigma_y^2}\right] \exp\left[\frac{2z_p^2 - h_v^2}{4\sigma_z^2}\right] \quad (\text{A.18})$$

$$i_{\infty t_E} = \sqrt{\left(\frac{t_E}{3}\right)^2 (1 + i_{\infty}^2) - 1} \quad \text{for } t_E > 3 \text{ minutes} \quad (\text{A.25})$$

$$i_{\infty t_E} = i_{\infty} \quad \text{for } t_E \leq 3 \text{ minutes}$$

$$\lambda \equiv \frac{\sqrt{\sigma_y \sigma_z}}{z_i} \quad (\text{A.19})$$

$$\lambda_o = \frac{0.12}{1 + 0.055 \frac{\Lambda}{2R}} \quad (\text{A.20})$$

$$\Lambda = 0.6z_p \exp \left[-\left(\frac{\sigma_z}{z_p} \right)^2 \right] \quad (\text{A.21})$$

$$h_v = [z_p^2 + 0.498\sigma_z^2]^{\frac{1}{2}} \quad (\text{A.22})$$

$$i = 0.316i_{\infty} \quad (\text{A.23})$$

$$i_p = 0.316i_{p\infty} \quad (\text{A.24})$$

For transient releases, i_p varies during the exposure, so we must choose an appropriate "exposure averaged" value for which to calculate the log standard deviation S_L for toxic load. For the case where no zero loads are observed, $\gamma_L = 1.0$ and it can be shown that for s_{nj} defined at each time step t_j by:

$$S_{nj}^2 = n^2 \ln(1 + i_{pj}^2) \quad (\text{A.26})$$

where i_{pj} is given by Equation A.24, that the exposure time averaged S_L is given by

$$S_L^2 = \frac{1}{N} \sum_{j=1}^N S_{nj}^2 \quad (\text{A.27})$$

Based on Equation A.8,

$$S_L^2 = n^2 \ln(1 + i_p^2) \quad (\text{A.28})$$

With S_L known from (A.27), the exposure averaged i_p can be solved from:

$$1 + i_p^2 = \exp\left(\frac{S_L^2}{n^2}\right)$$

In applying these equations, it was found that for downwind distances off the plume centreline ($y>0$), Equation (A.10) posed computational problems since γ tended to zero. In fact, the expression for $\bar{L}$ becomes indeterminate under these circumstances, so an alternate calculation for $\bar{L}$ was adopted:

$$\bar{L} = \bar{L}_0 \frac{\left[i_o^2 + \exp\left(\frac{-\gamma^2}{2\sigma_y^2}\right) \right]^n}{[i_o^2 + 1]^{n-1} \left[1 + i_o^2 \exp\left(\frac{\gamma^2}{2\sigma_y^2}\right) \right]} \quad (\text{A.26})$$

where i_o = value of i at the plume centreline ($y=0$)

$\bar{L}_0$ = value of $\bar{L}$ at the plume centreline ($y=0$)

Equation (A.26) was derived from the crosswind variations of γ and $\bar{C}_p$ reported by Wilson (1986).

The calculation procedure goes as follows:

- (a) For the plume centreline ($y=0$) apply the closed equation set (A.2) through (A.25). The value of i from Equation (A.23) is stored as i_o and the value of $\bar{L}$ from Equation (A.10) is stored as $\bar{L}_0$.
- (b) Following the centreline calculations, the calculations for off the plume centreline ($y>0$) are performed. Equation (A.10) is replaced by Equation (A.26) for $\bar{L}$, and Equation (A.16) for γ is strictly no longer required for determining L_M and S_L . Of course, the effect of γ is present in $\bar{L}_0$ and hence indirectly is present in all the subsequent $\bar{L}$.

It is worthy of note emphasis that $\bar{L} = \bar{L}(x,y)$, $i = i(x,y)$ and $i_p = i_p(x)$. Hence $S_L = S_L(x)$ and $L_M = L_M(x,y)$. Since the dependence on y in all of the equations in this Appendix is symmetrical, one need only calculate L_M for $y>0$.

The independent input variables which determine L_M and S_L are:

t_e = exposure time in minutes to downwind loads. For steady releases, this time is determined by the expected persistence of meteorological conditions (taken as 60 minutes in this study). For transient releases, the exposure time is implicitly present in the GASCON2 output.

n = power in the definition of toxic load. This is a probit parameter determined from lethality experiments on animals (see Section 4.6).

The following inputs are known inside the GASCON2 model calculations:

z_p = plume height
 σ_y = lateral plume standard deviation
 σ_z = vertical plume standard deviation
 z_i = mixed layer height
 R = radius of jet/plume 1 second after release
 x = downwind distance
 y = cross wind distance
 t_E = event time

N.L.C. - B.N.C.



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